libEnsemble: A Library for Managing Ensembles of Calculations

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- `libEnsemble` uses a manager to allocate work to various workers.
- A `libEnsemble` worker is the smallest indivisible unit to perform

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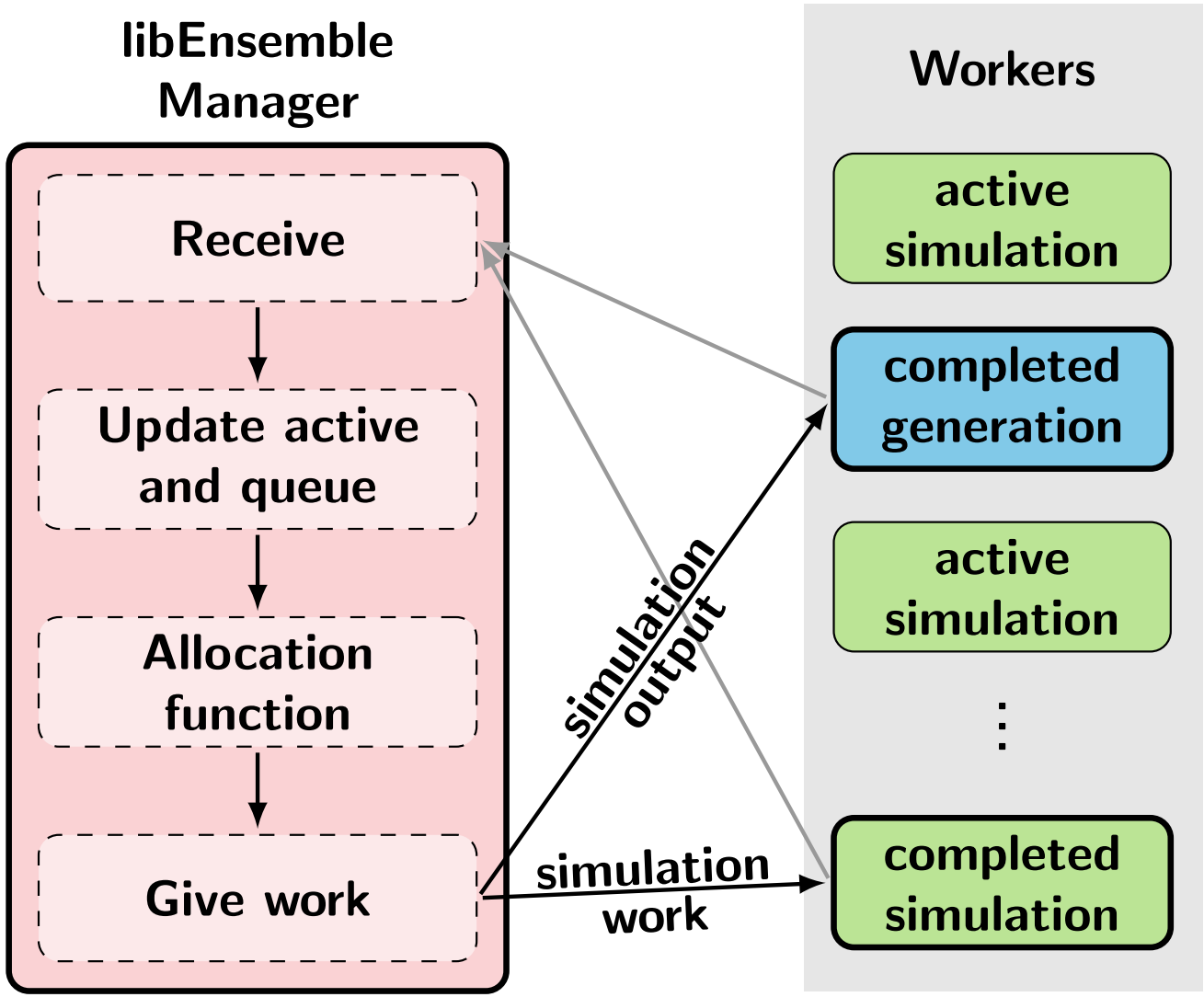
`sim_f`: Evaluates a simulation (i.e., user-defined function) using input defined by `gen_f`.

`alloc_f`: Decides whether (or not) `sim_f` or `gen_f` should be called (and with what input/resources) as workers become available.

`libEnsemble` dependencies

- Python 2.7, 3.4 or above.
- An MPI 1.x/2.x/3.x implementation (e.g., MPICH or OpenMPI) built with shared/dynamic libraries.
- mpi4py v2.0.0 or above.
- NumPy v1.10 or above.

libEnsemble overview



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- (*) Execution on multiple LCFs
- (*) Thousands of concurrent workers

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- Don't have to write your own kills, just complete `libEnsemble` templates.
- Want to add concurrency to a generator (e.g., multiple local optimizers.)

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Swift: (the parallel scripting language)
- "Can run million programs, thousands at a time, launching hundreds per second."
- Require writing your generators in Swift's scripting language.
- Difficult to tightly couple generation of inputs and future/active running simulations.

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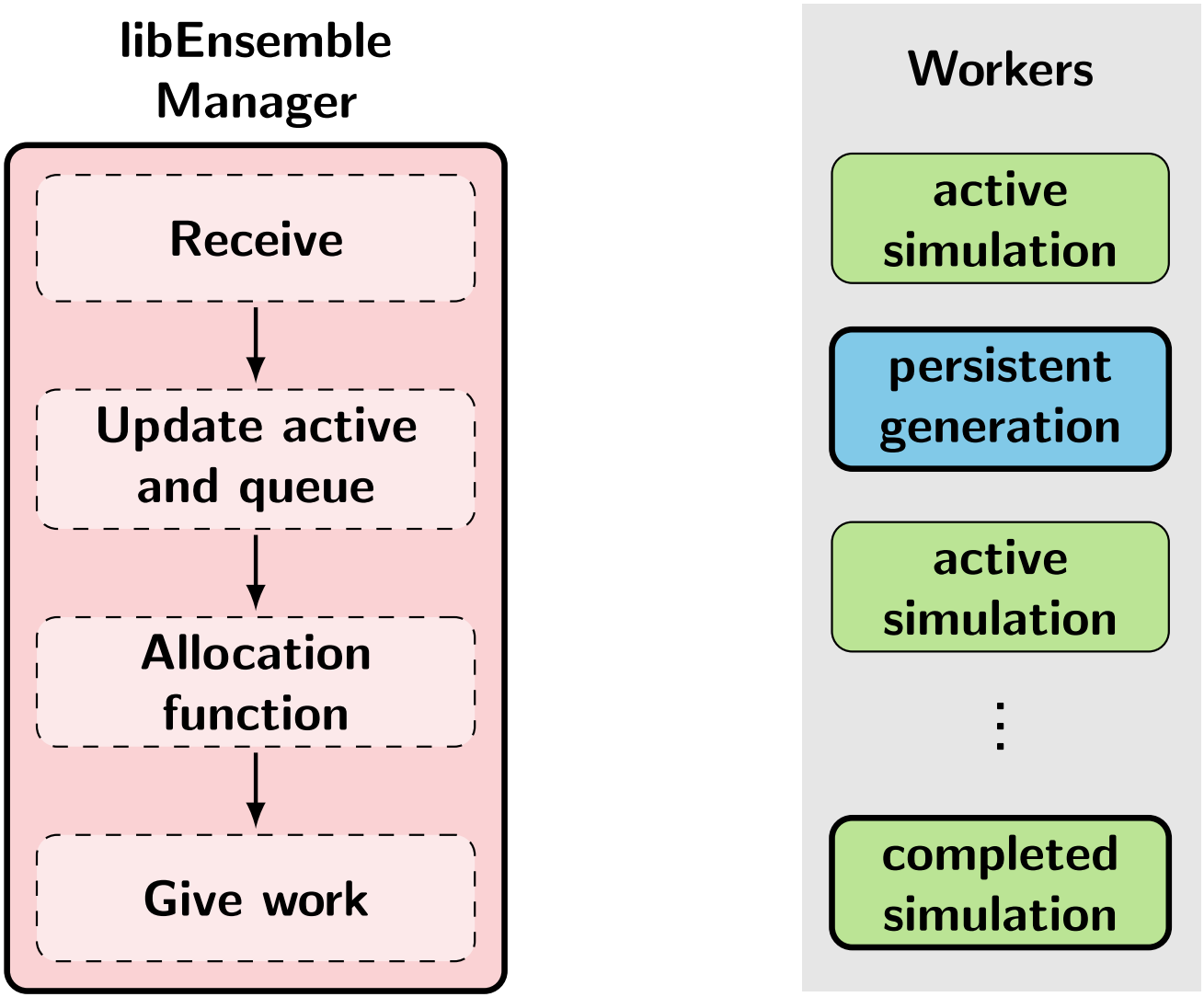

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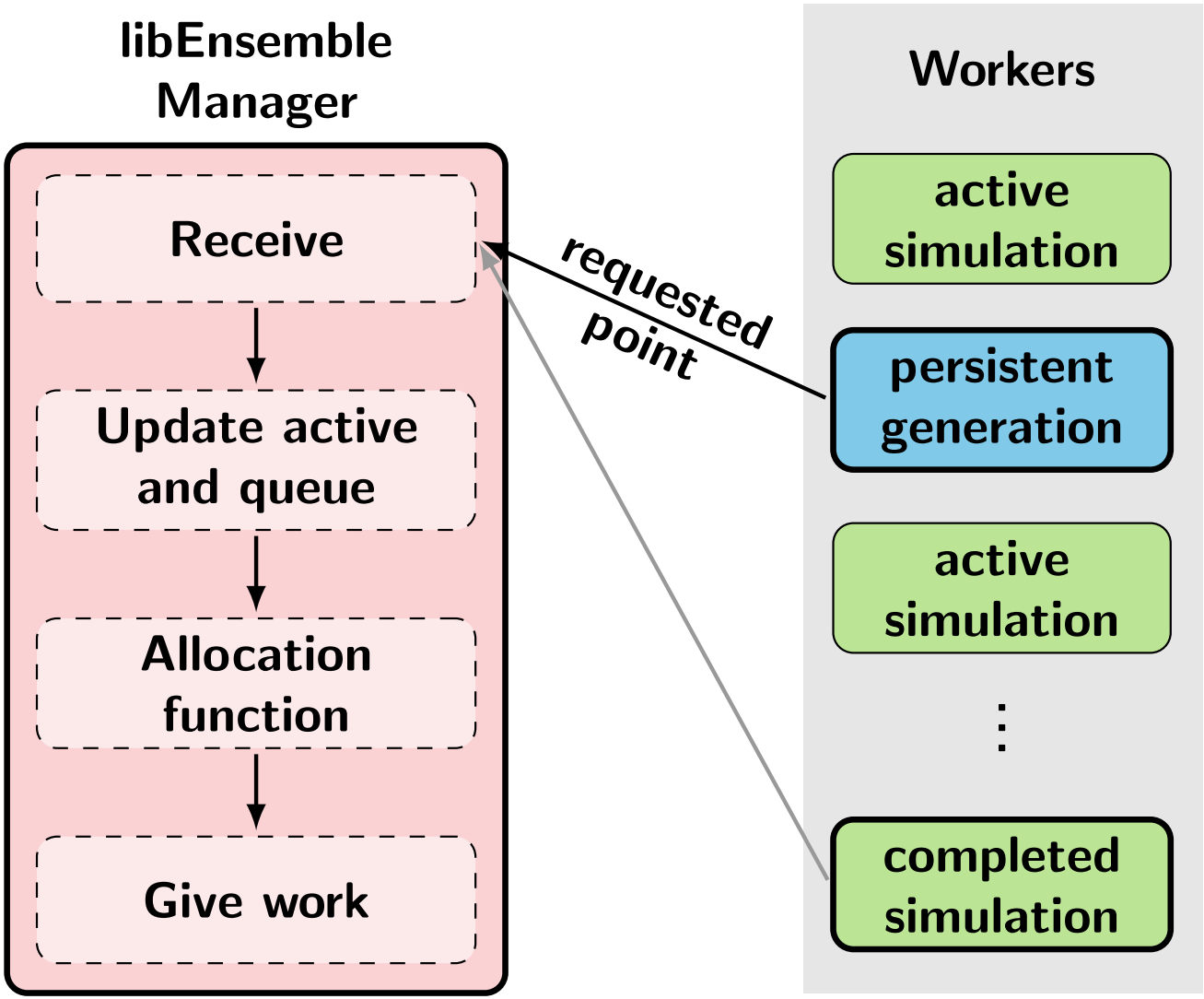

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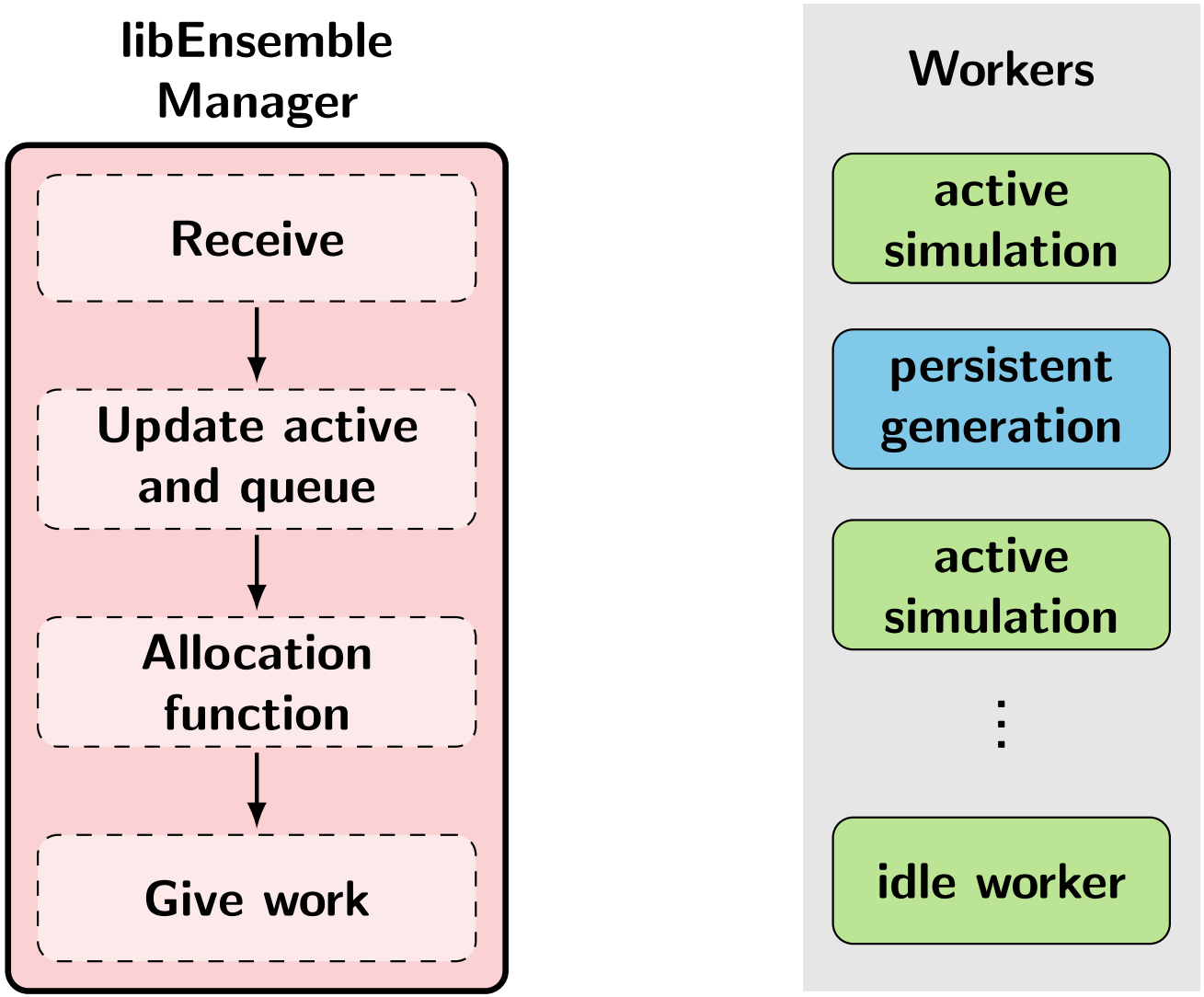

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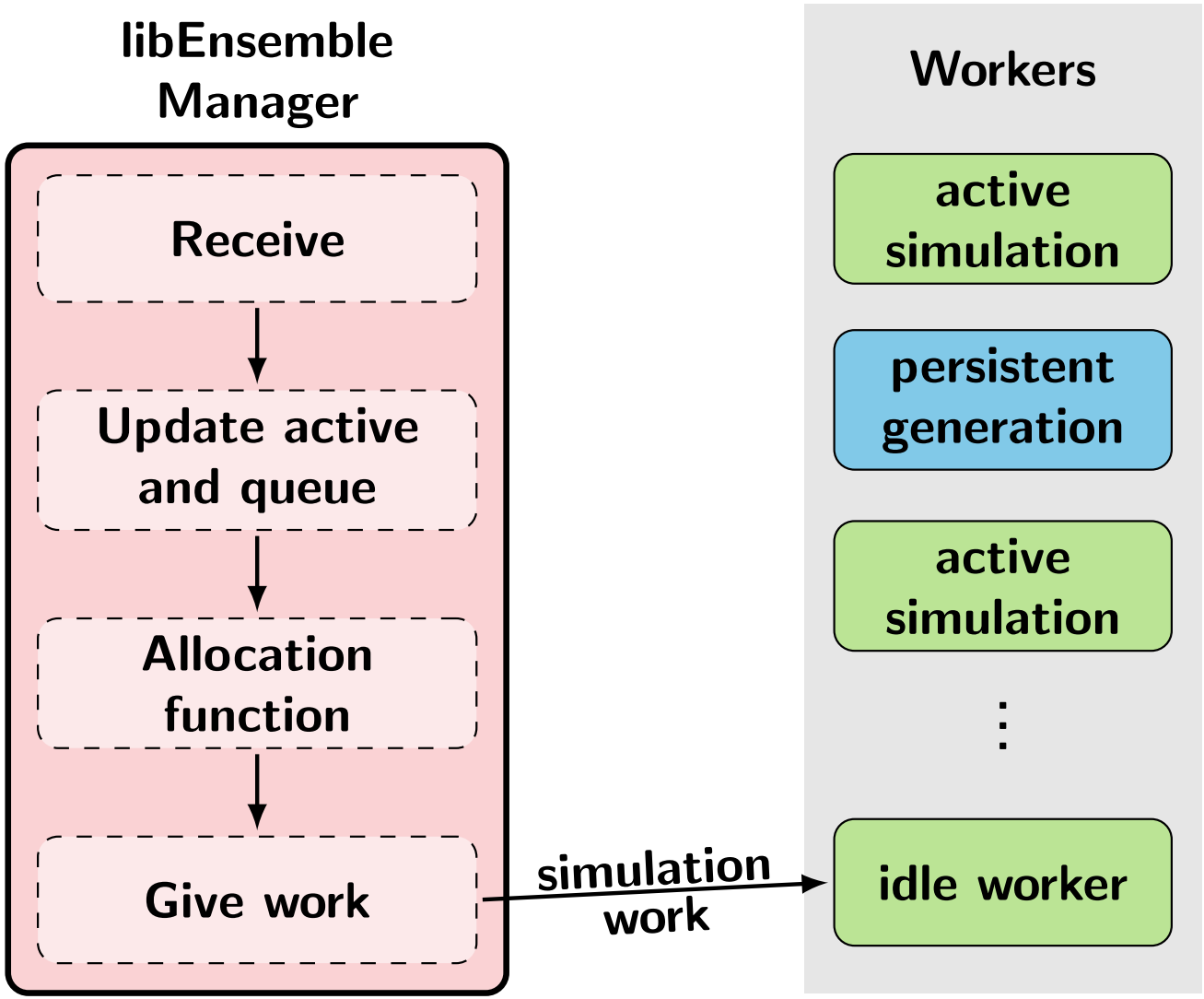

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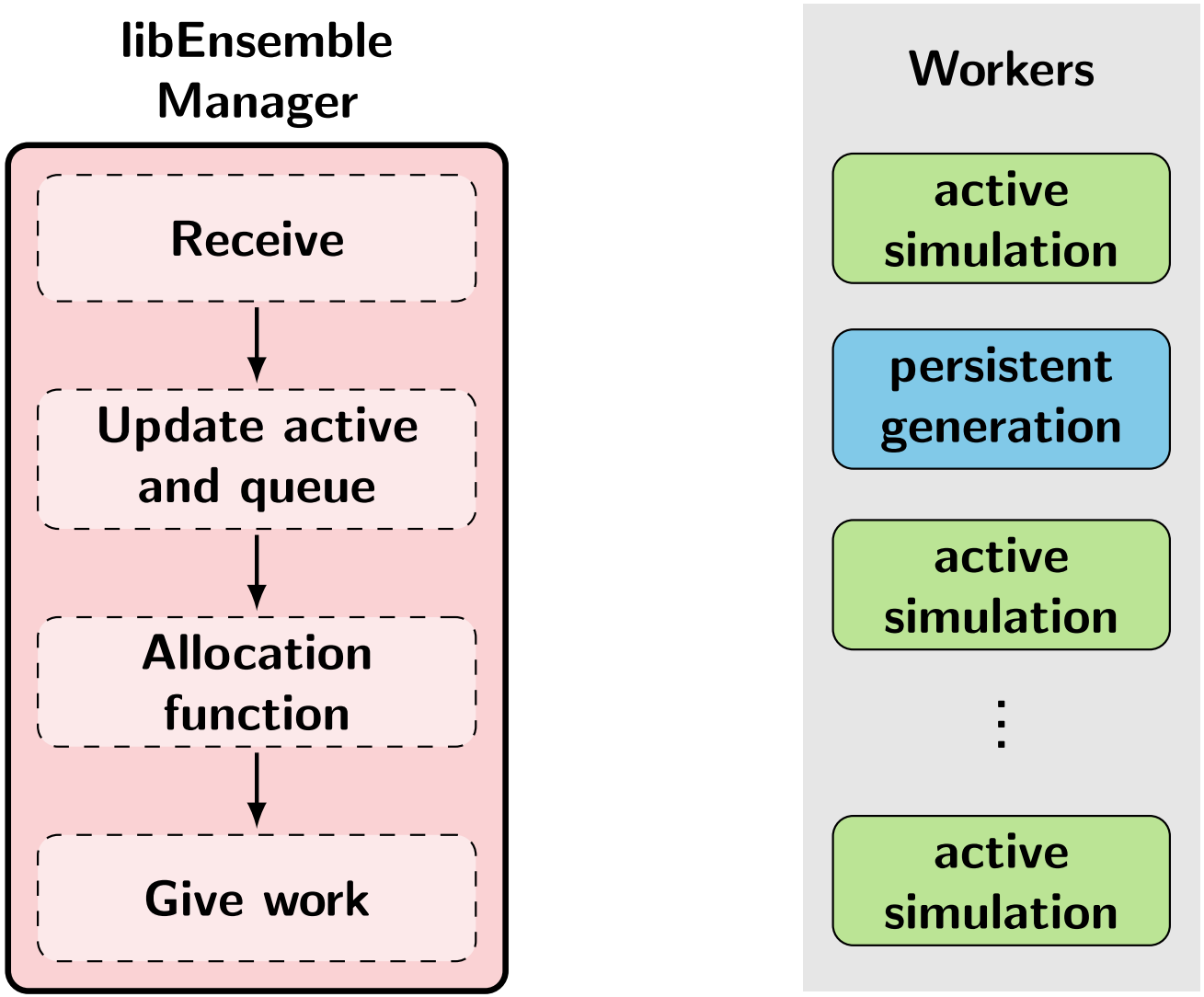

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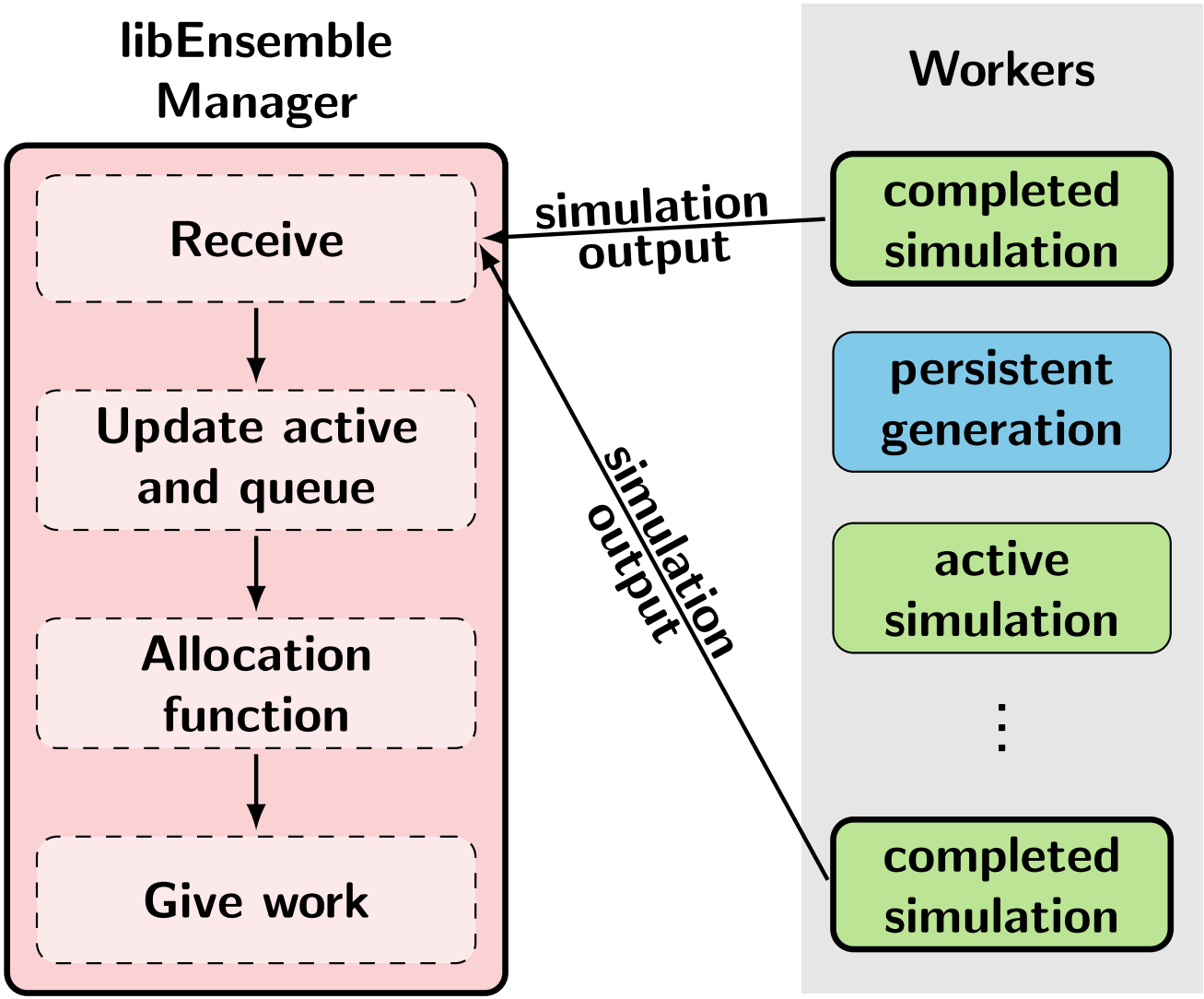

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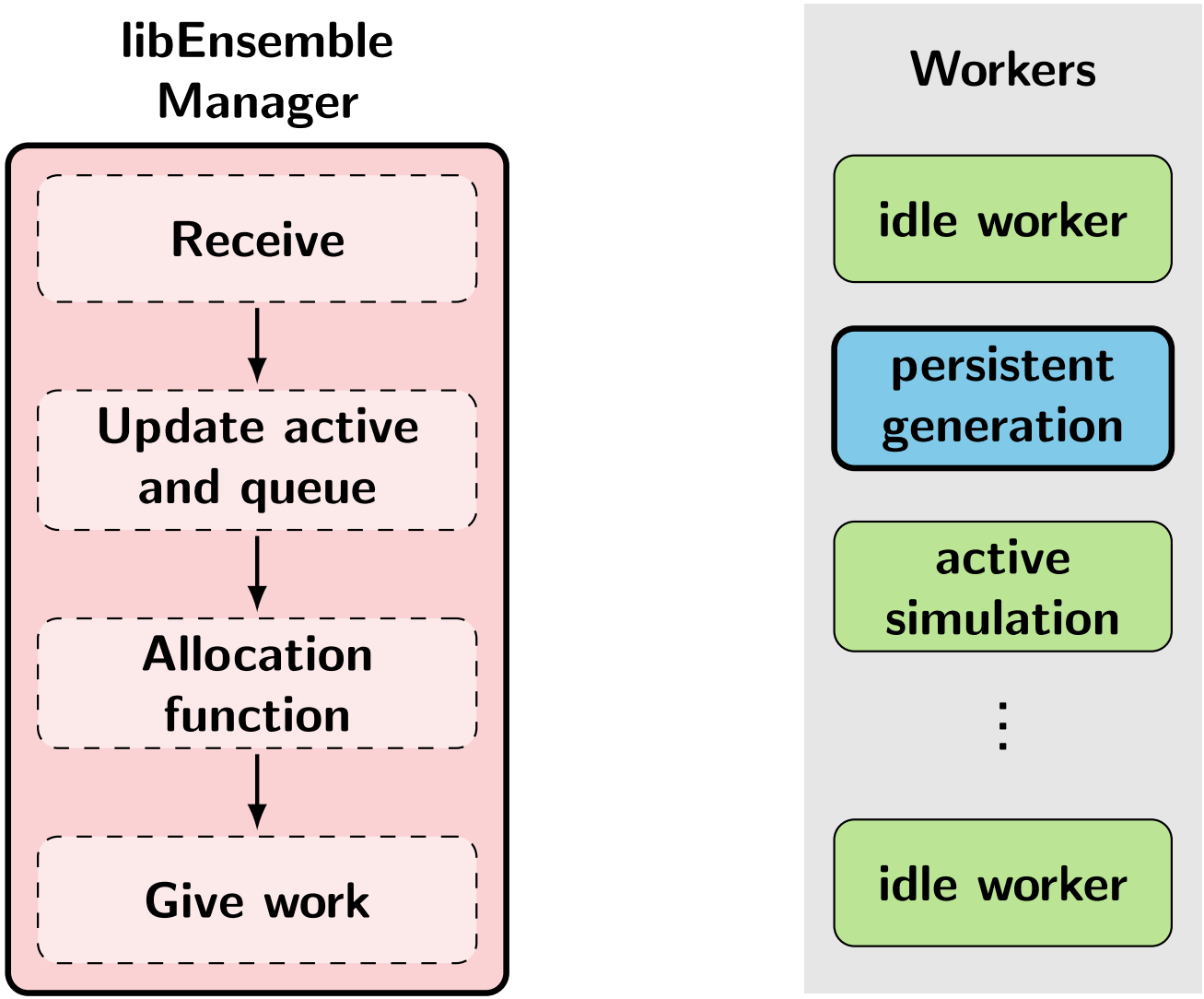

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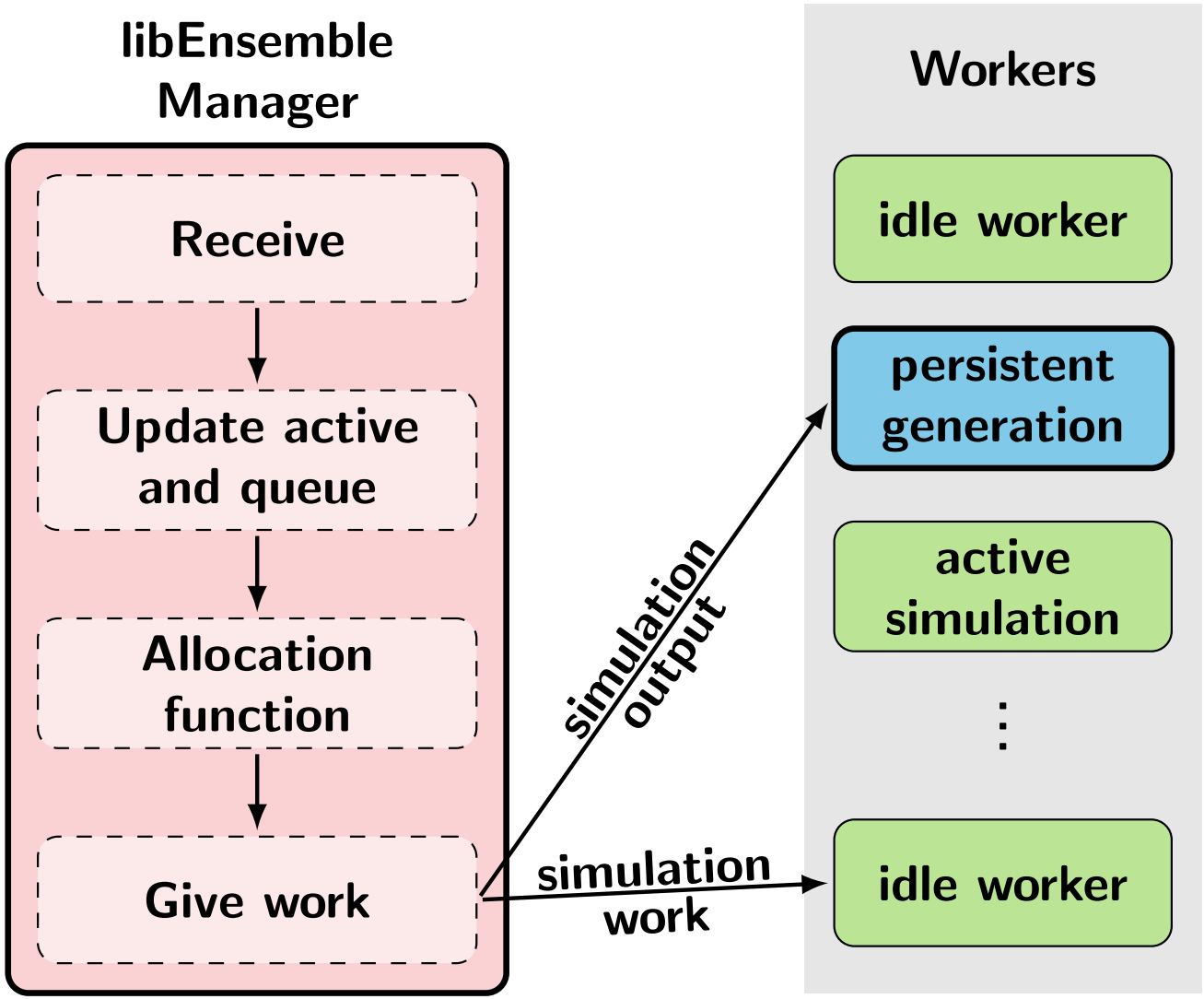

Timing `libEnsemble` overhead

Time for `libEnsemble` to sample/evaluation 30$\times$(workers) points

Tons of system-dependent caveats

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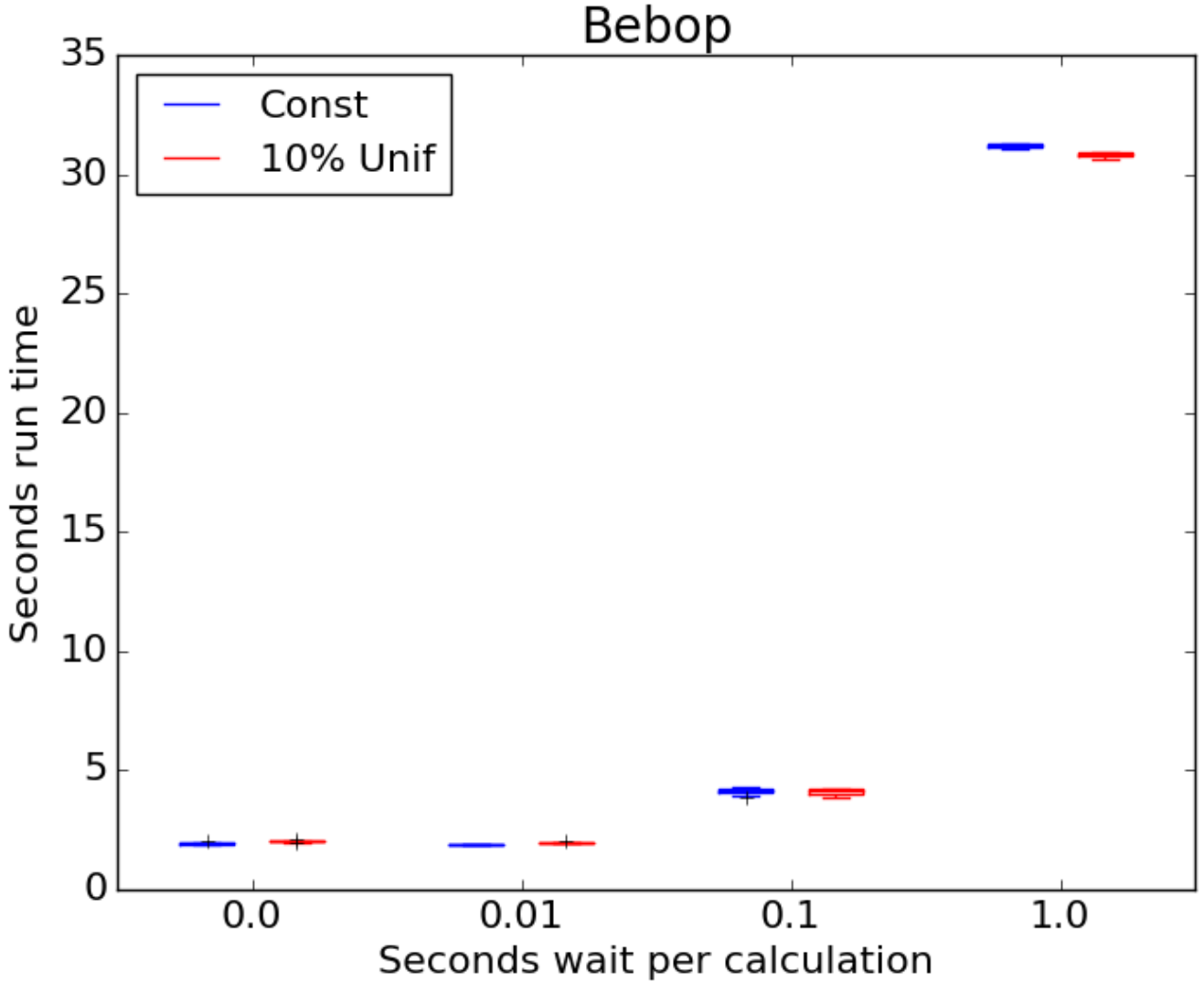
Time for `libEnsemble` to sample/evaluation 30×(workers) points

32 nodes × 36 cores = 1152-1 workers



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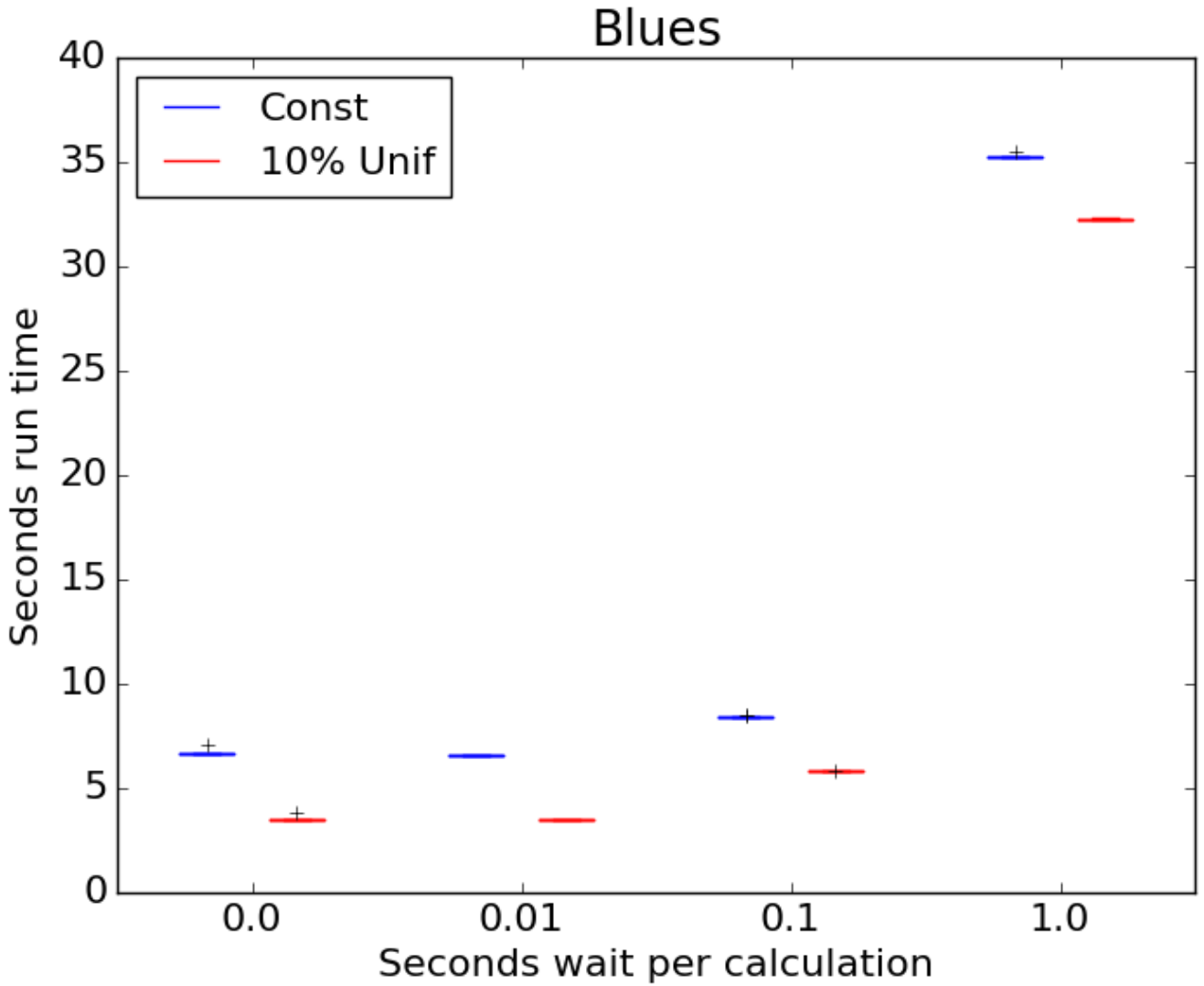
64 nodes × 16 cores = 1024-1 workers



Use cases

- A user wants to optimize a function that depends on a simulation.
- The simulation is already using parallel resources, but not a large fraction of some computer.
- `libEnsemble` can coordinate the concurrent evaluation of the simulation `sim_f` at various parameter values and `gen_f` would return candidate parameter values (possibly after each `sim_f` output).

Use cases

- A user has a `gen_f` that produces different meshes to be used within a `sim_f`.
- Given the `sim_f` output, `gen_f` will refine a mesh or produce a new mesh.
- `libEnsemble` can ensure that the calculated meshes can be used by multiple simulations without requiring movement of data.

Use cases

- A user wants to evaluate a simulation `sim_f` at parameters sampled from a set of parameter values.
- Many parameter sets will cause the simulation to fail.
- `libEnsemble` can stop unresponsive evaluations, and recover computational resources for future evaluations.
- `gen_f` can update the sampling after discovering regions where evaluations of `sim_f` fail.

Use cases

- A user has a simulation `sim_f` that requires calculating multiple expensive quantities, some of which depend on other quantities.
- `libEnsemble` can observe intermediate quantities in order to stop related calculations and preempt future calculations associated with a poor parameter values.

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Naturally, combinations of use cases is supported as well.

Problem setup

- We want to identify distinct, "high-quality", local minimizers of

$$\begin{aligned} \text{minimize } & f(x) \\ & l \leq x \leq u \\ & x \in \mathbb{R}^n \end{aligned}$$

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- Derivatives of f may or may not be available.
- The simulation f is likely using parallel resources, but it does not utilize the entire machine.

Global optimization is difficult

Theorem (Törn and Žilinskas, *Global Optimization*, 1989)

An algorithm converges to the global minimum of any continuous f on a domain $\mathcal{D}$ if and only if the algorithm generates iterates that are dense in $\mathcal{D}$.

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The theory can be more than merely checking that a method generates iterates which are dense in the domain.

Multistart Methods

Given some local optimization routine $\mathcal{L}$:

Algorithm 1: General Multistart

for $k = 1, 2, \ldots$ **do**
- Evaluate f at N points drawn from $\mathcal{D}$
- Start $\mathcal{L}$ at some set (possibly empty) of previously evaluated points

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- Which points should start runs?
- If resources are limited, how should points from each run receive priority?
- Ideally, only one run is started for each minima.
- Exploring by sampling. Refining with $\mathcal{L}$.

Multi-Level Single Linkage

- $f \in C^2$, with local minima in the interior of $\mathcal{D}$, and the distance between these minima is bounded away from zero.
- $\mathcal{L}$ is strictly descent and converges to a minimum (not a stationary point).
- $$r_k = \frac{1}{\sqrt{\pi}} \sqrt[n]{\Gamma\left(1 + \frac{n}{2}\right) \mathrm{vol}\left(\mathcal{D}\right) \frac{\sigma \log kN}{kN}} \tag{1}$$

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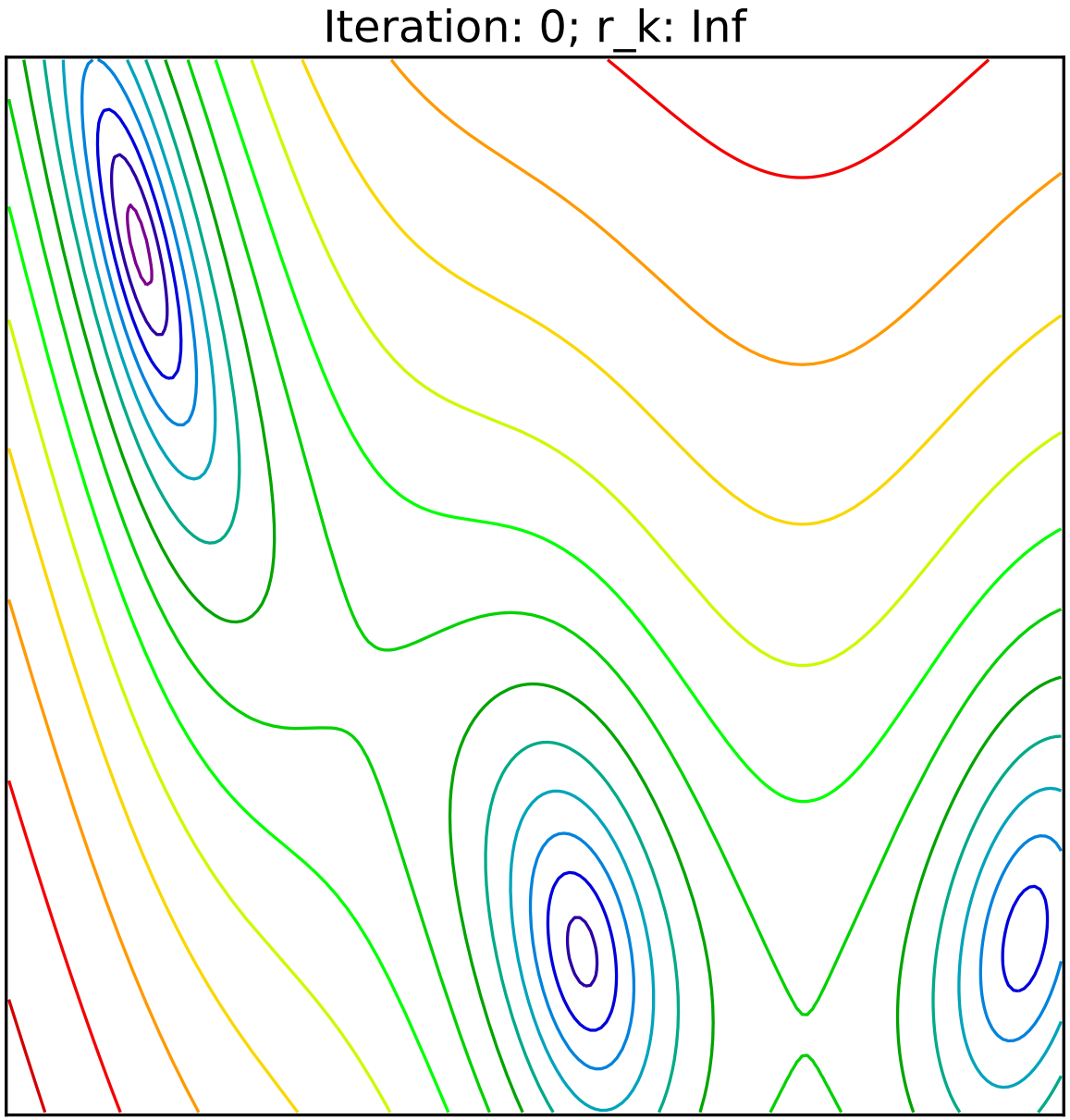
If r_k is defined by (1) with $\sigma > 4$, even if the sampling continues forever, the total number of local searches started is finite almost surely.

APOSMM



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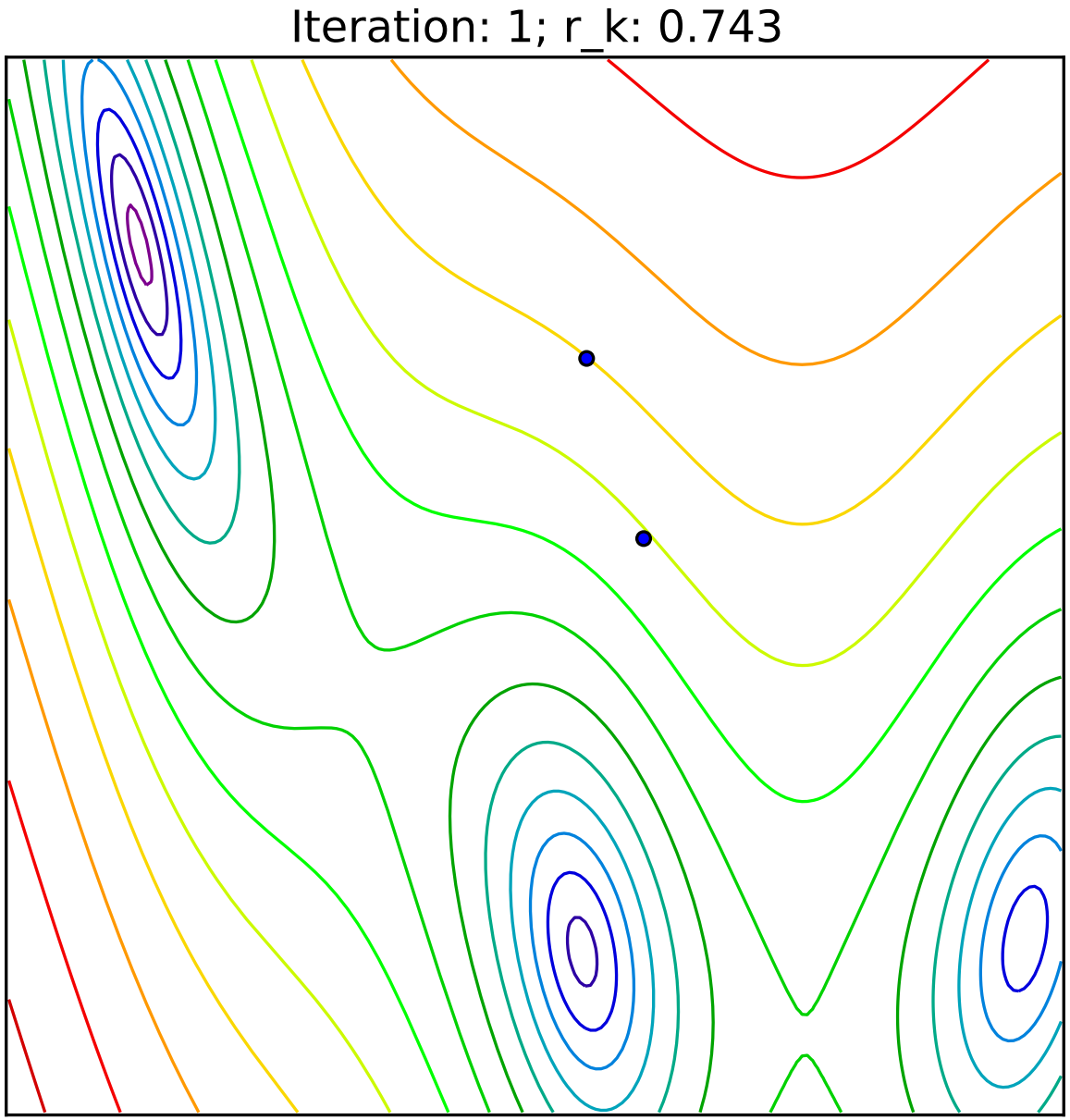

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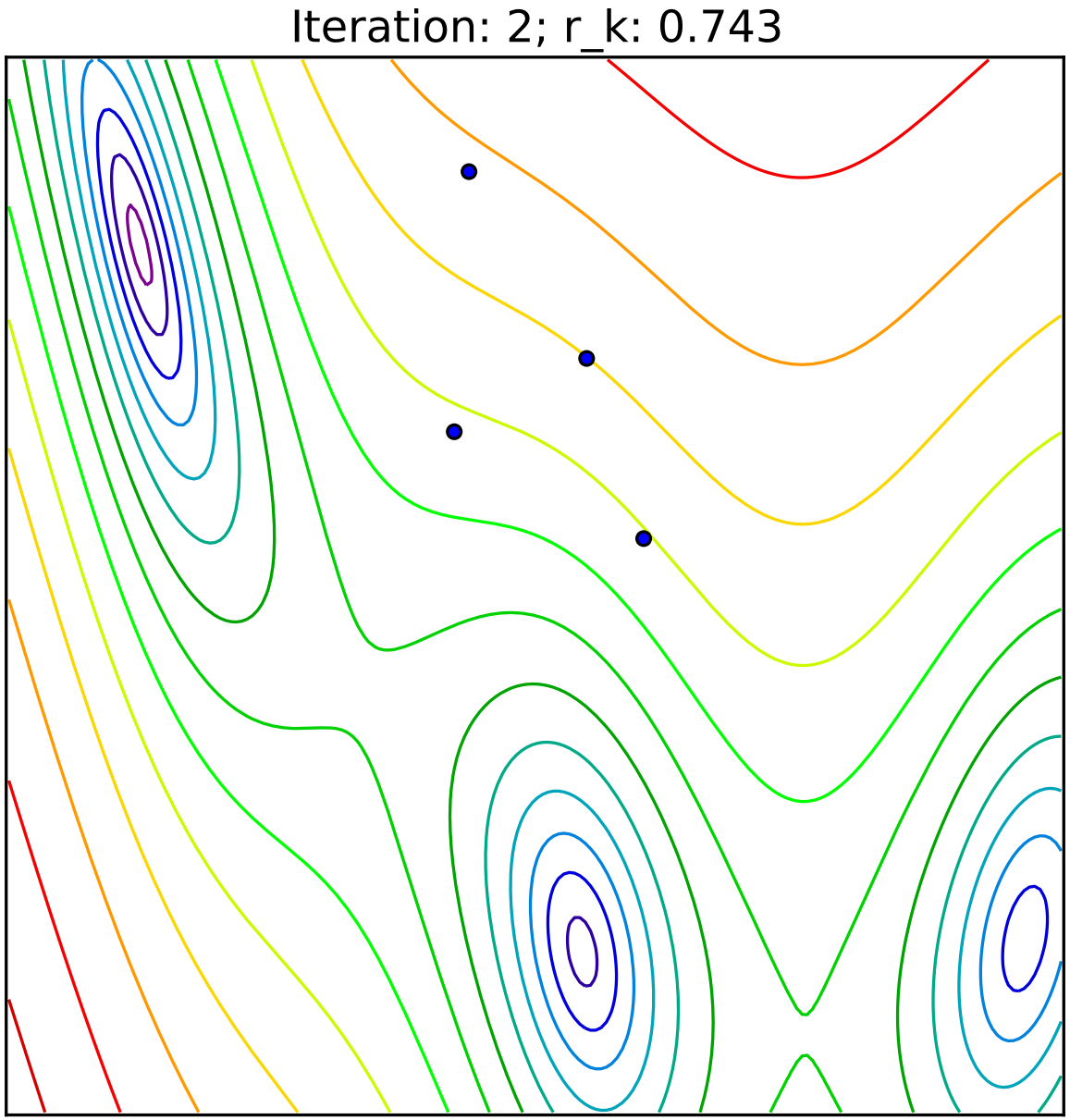

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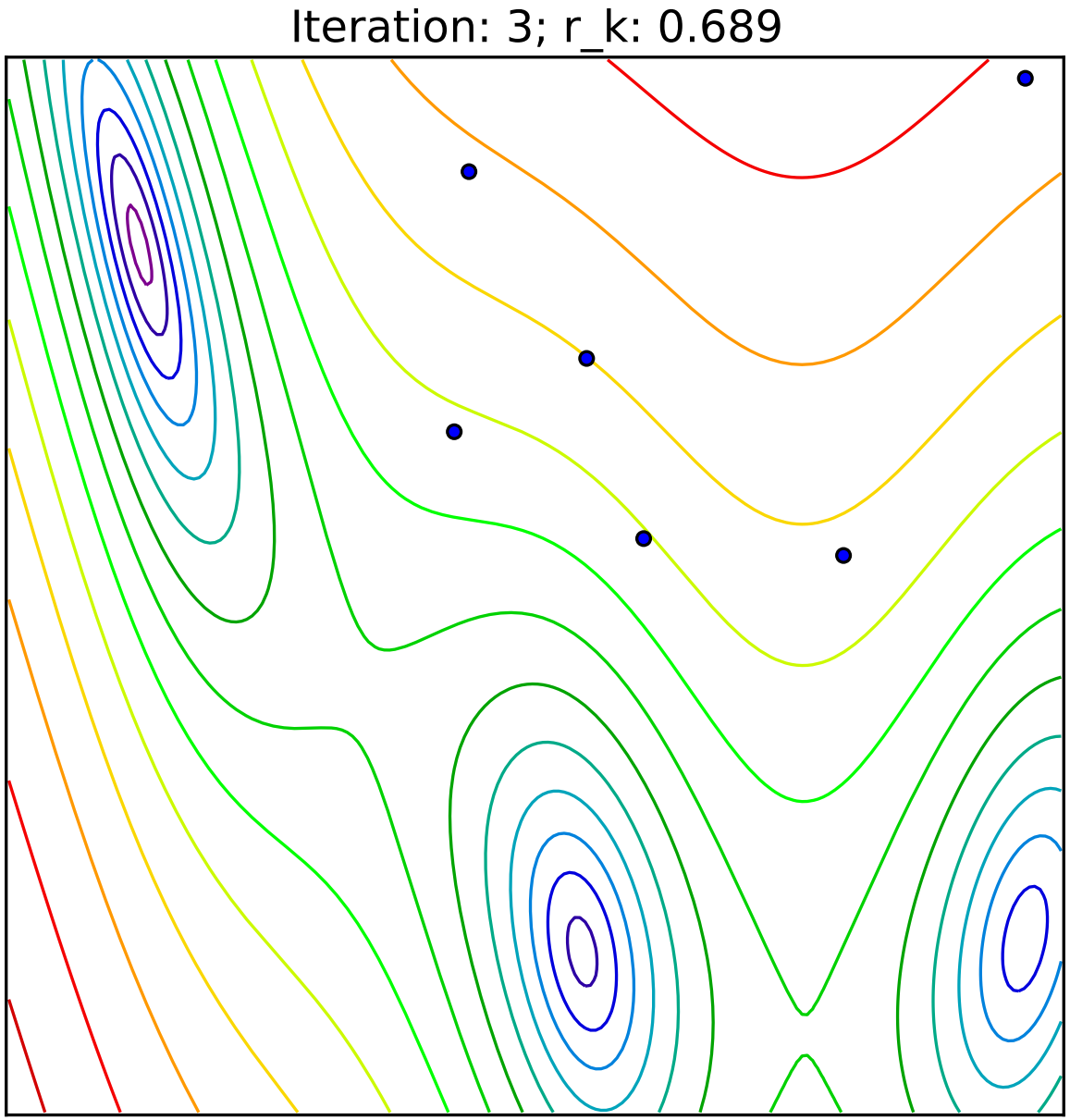

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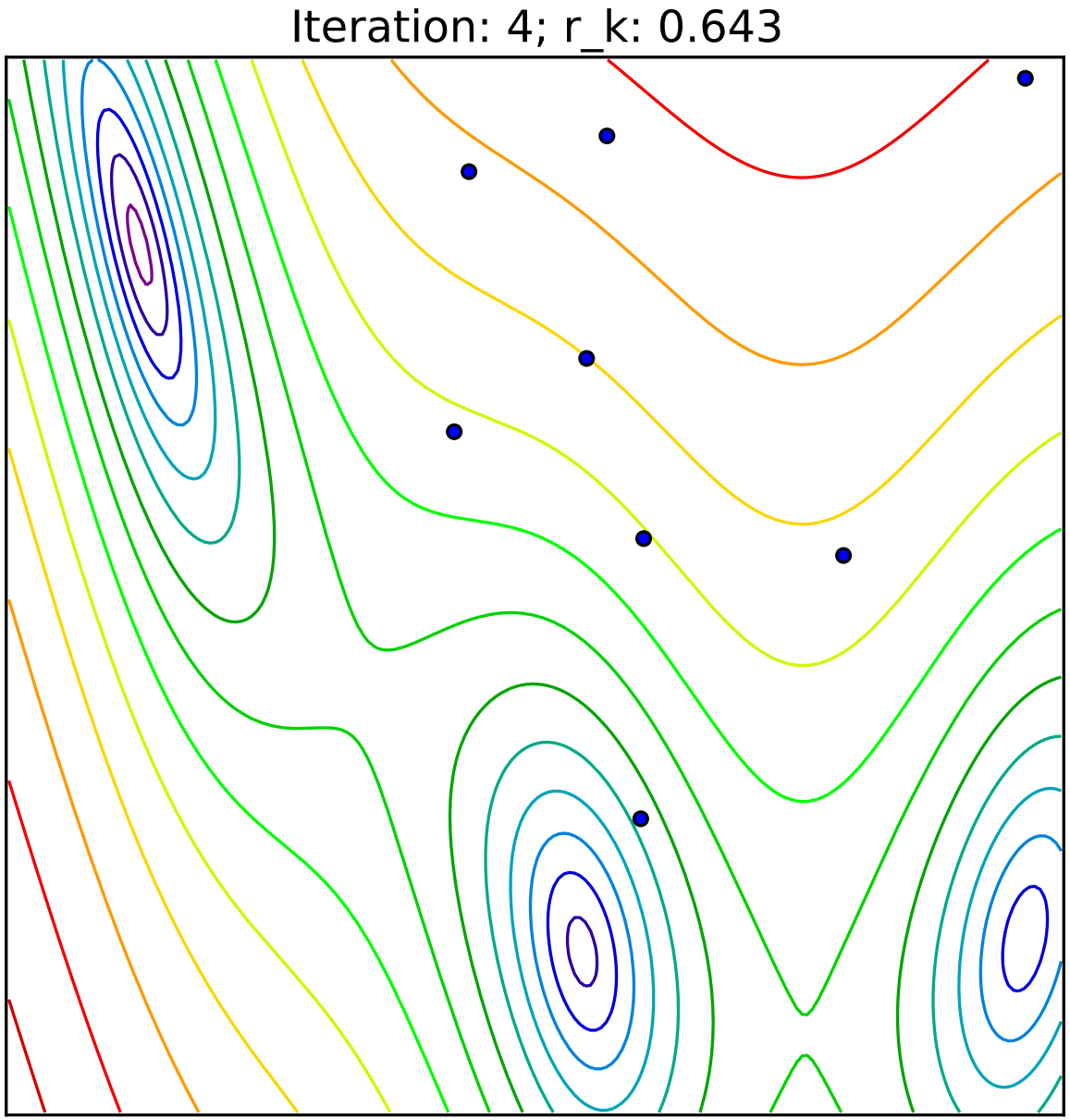

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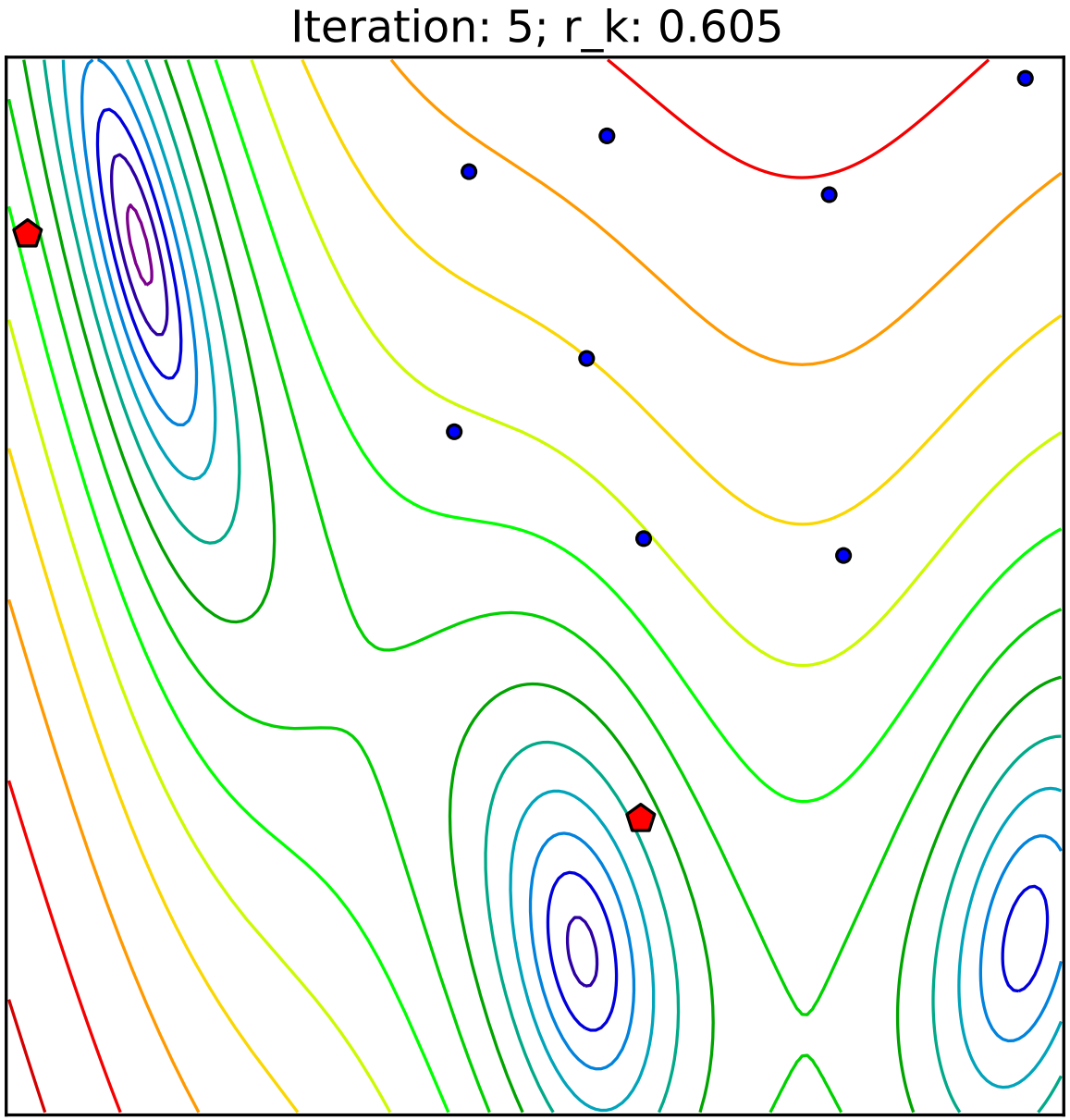

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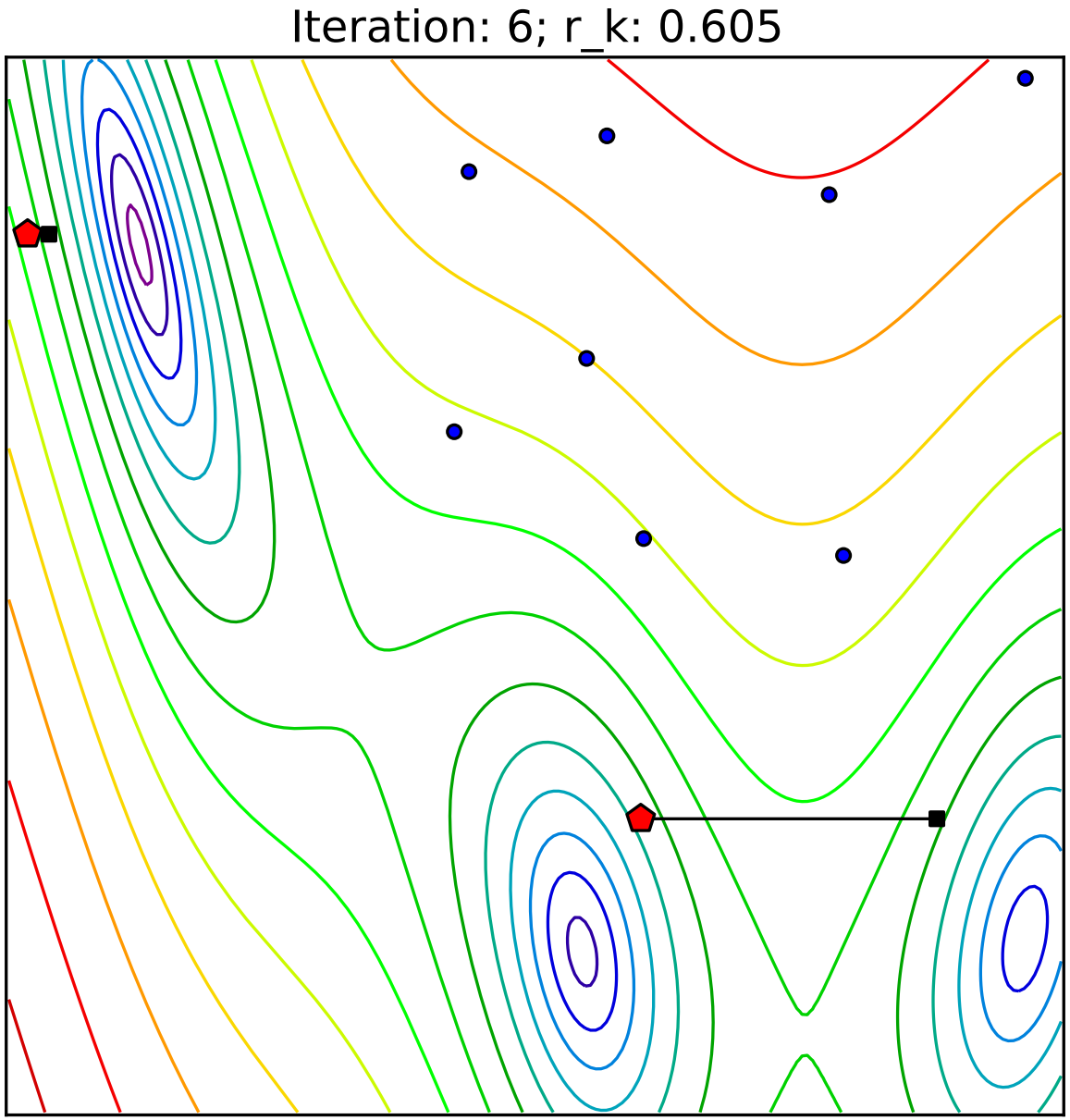

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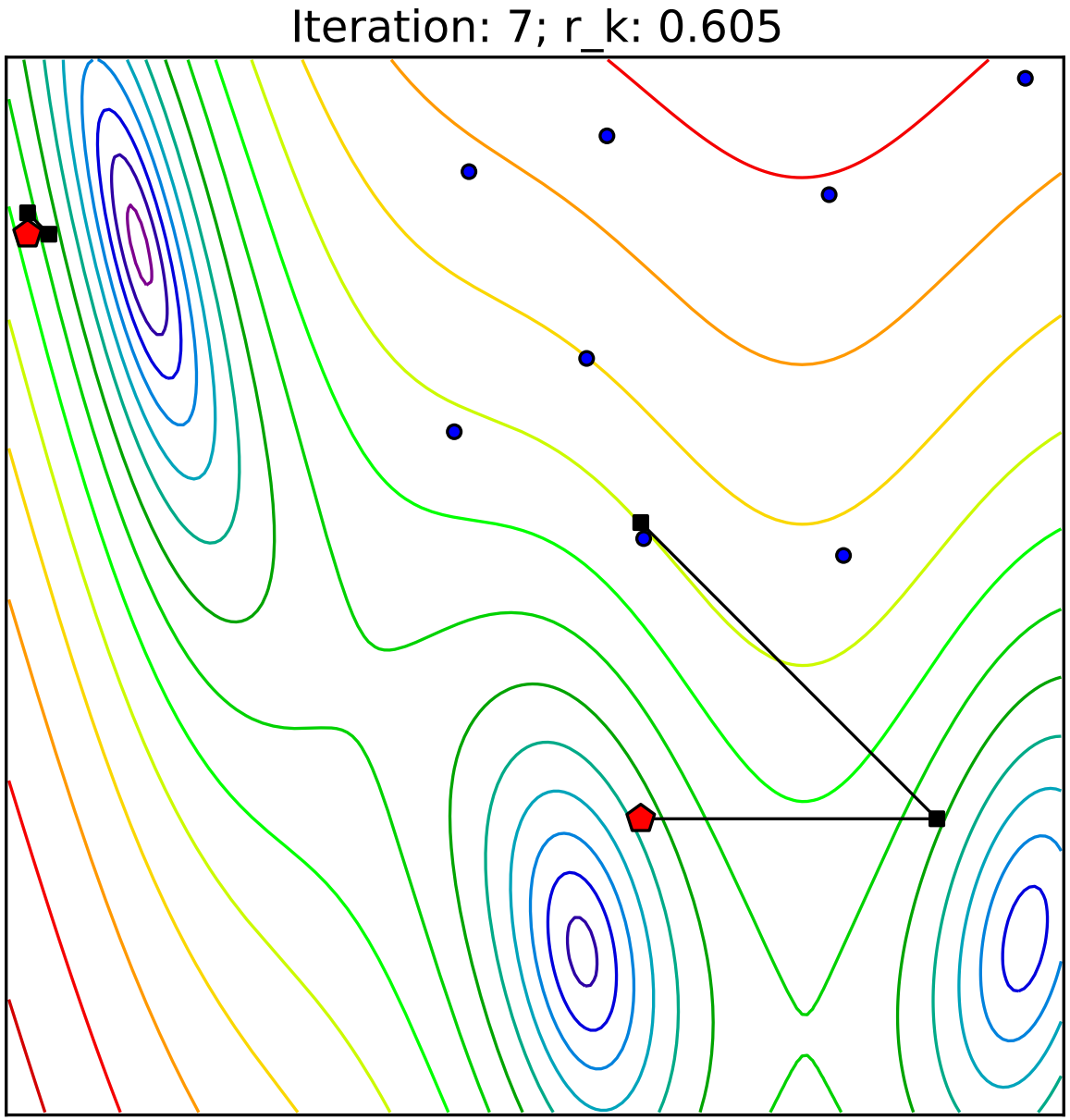

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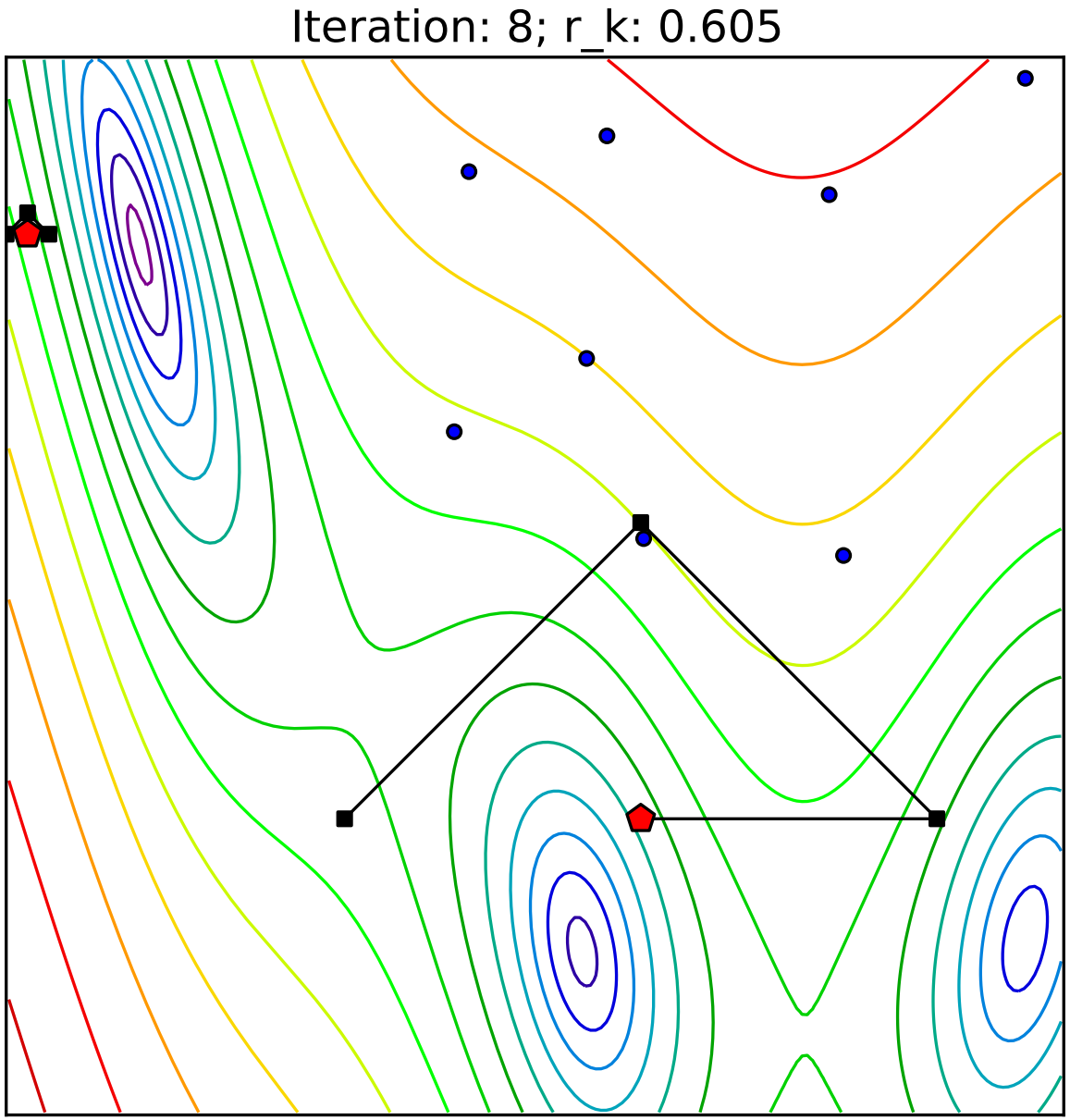

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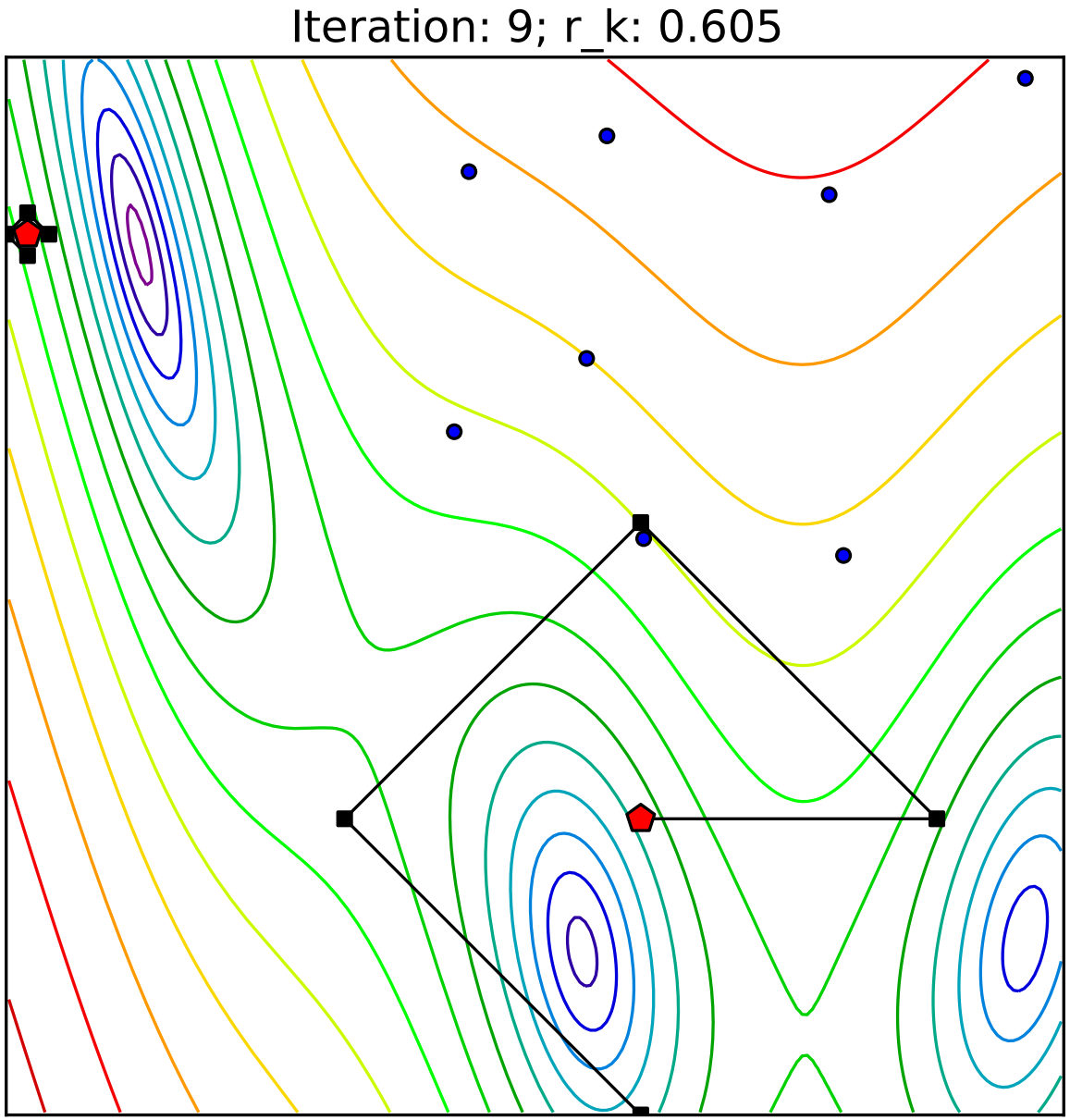

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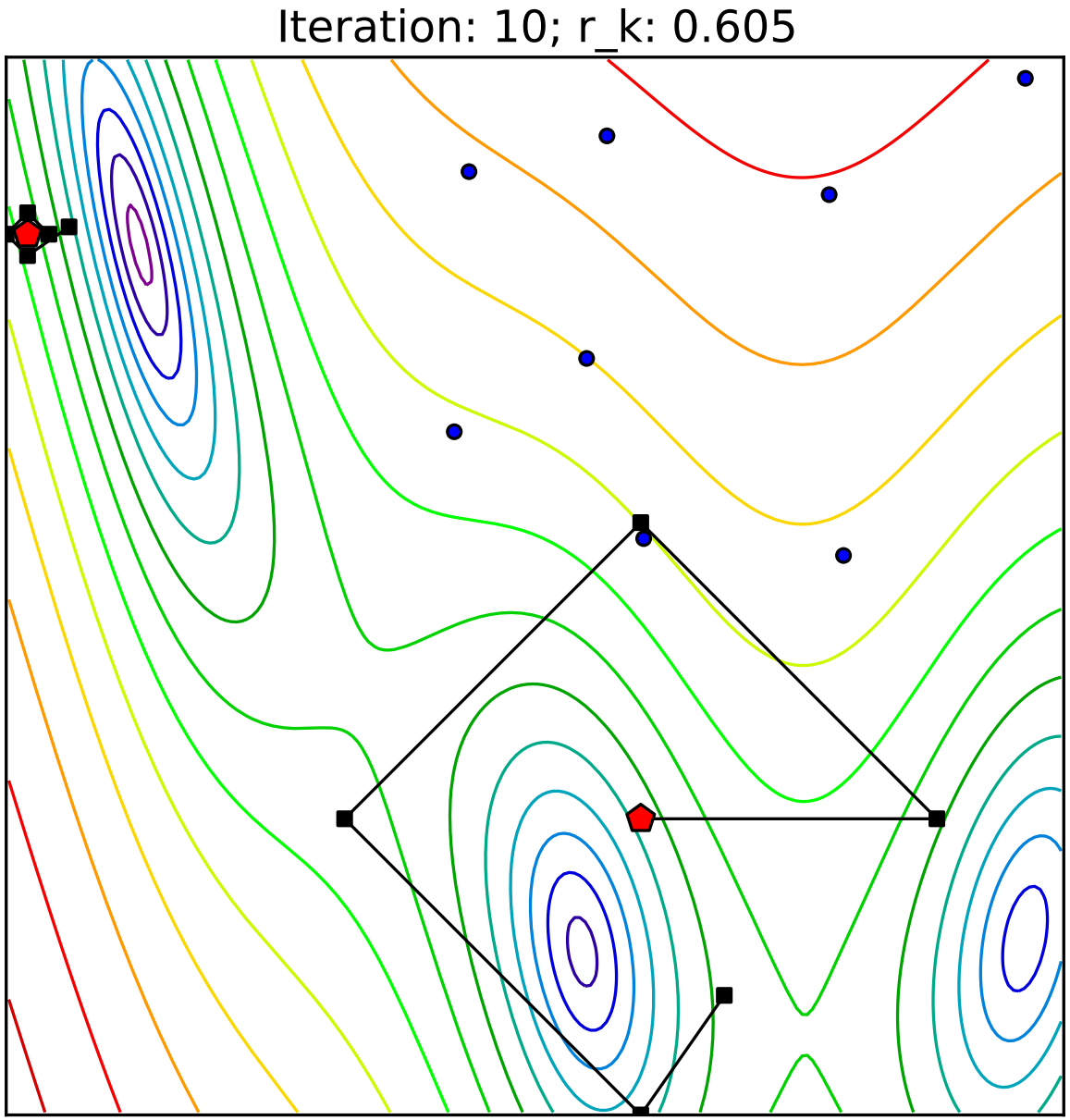

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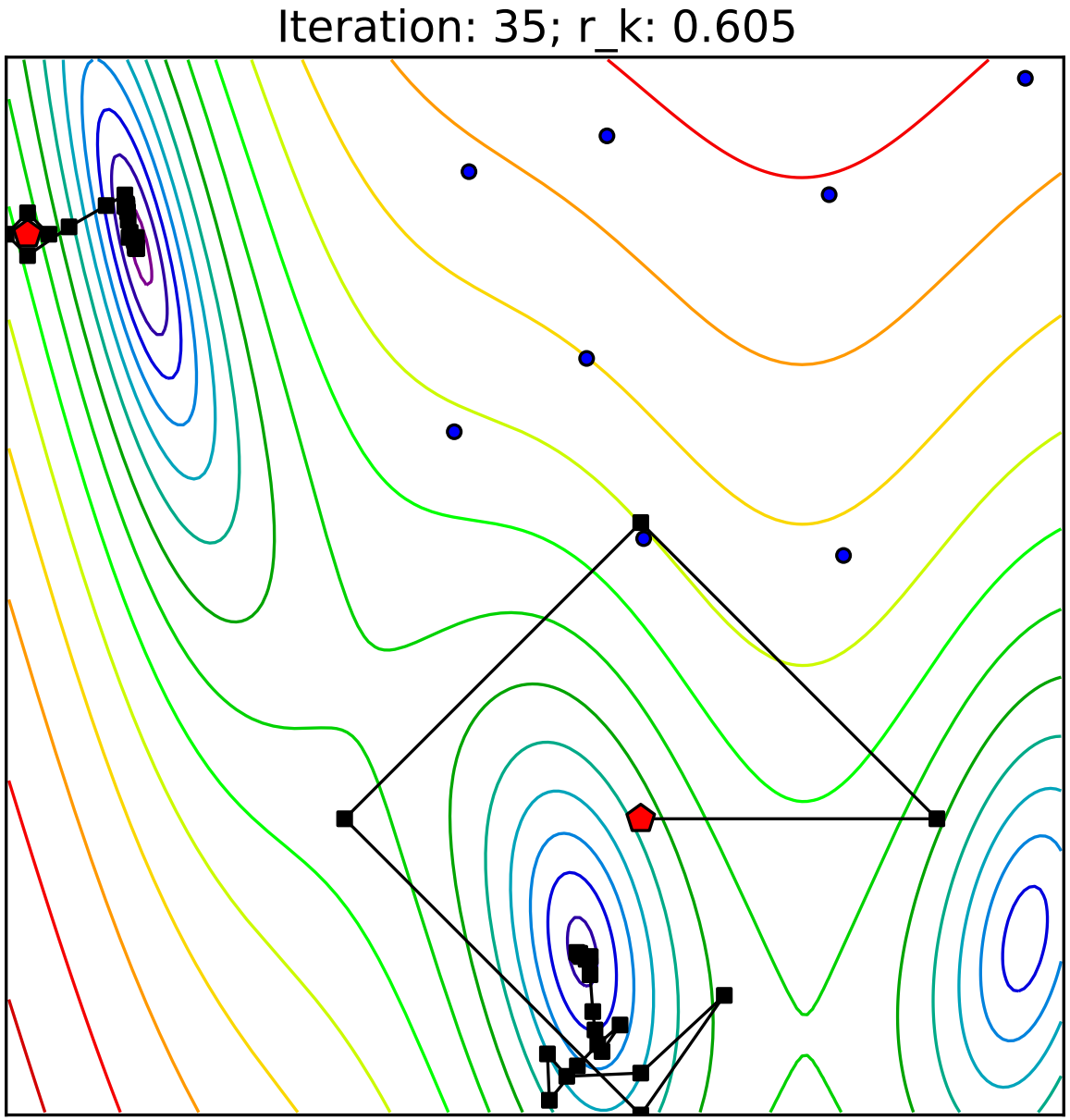

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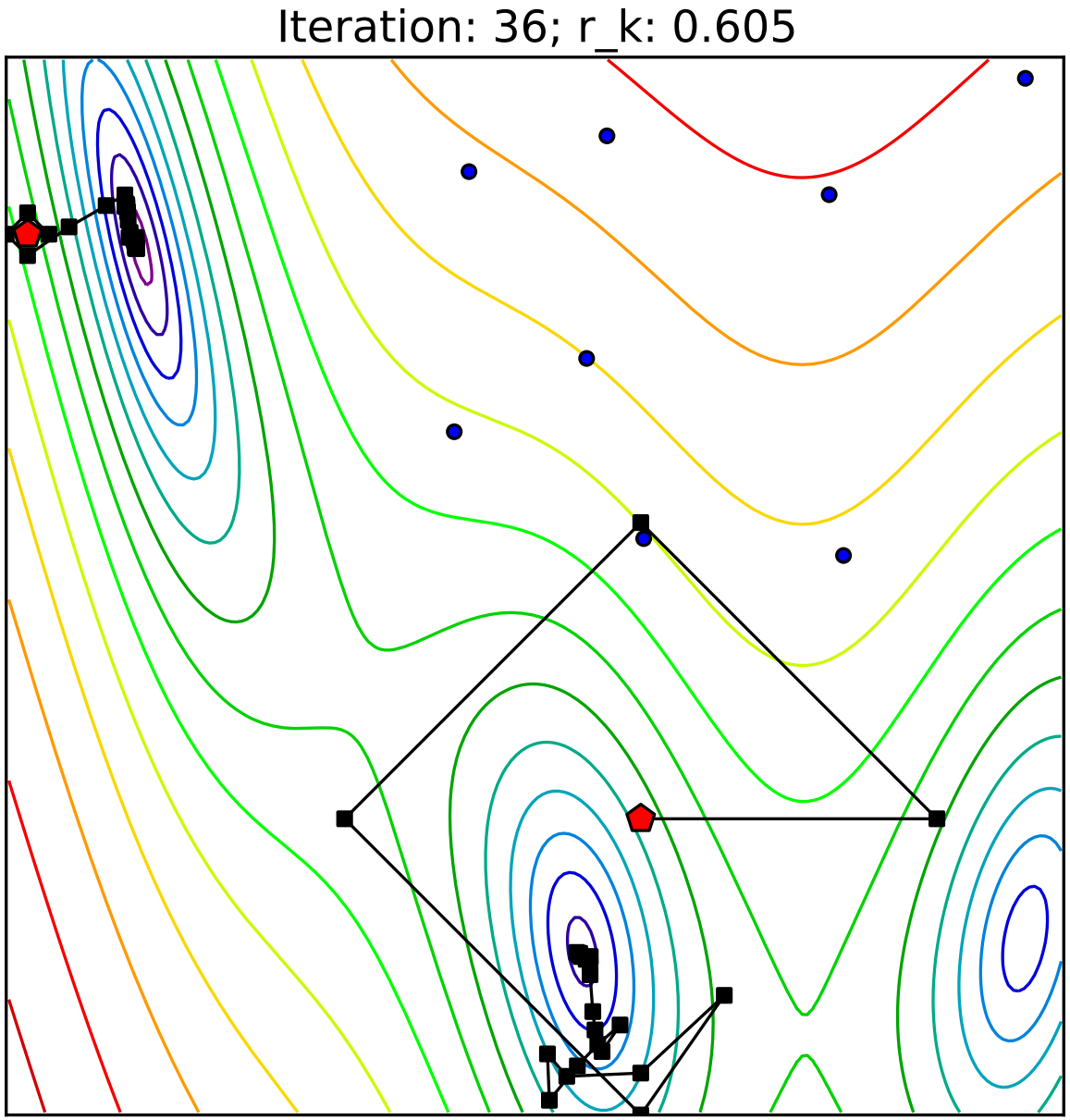

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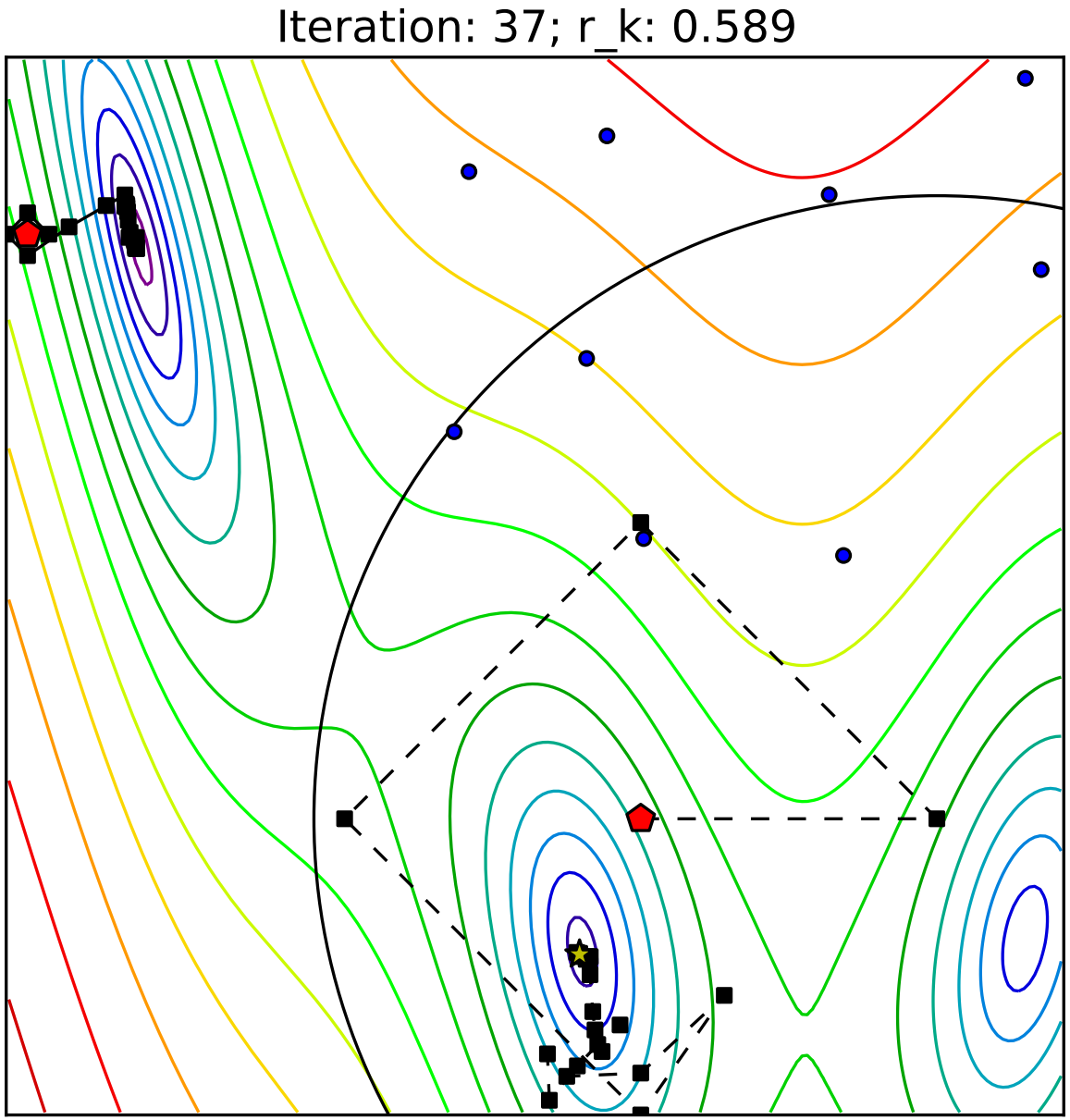

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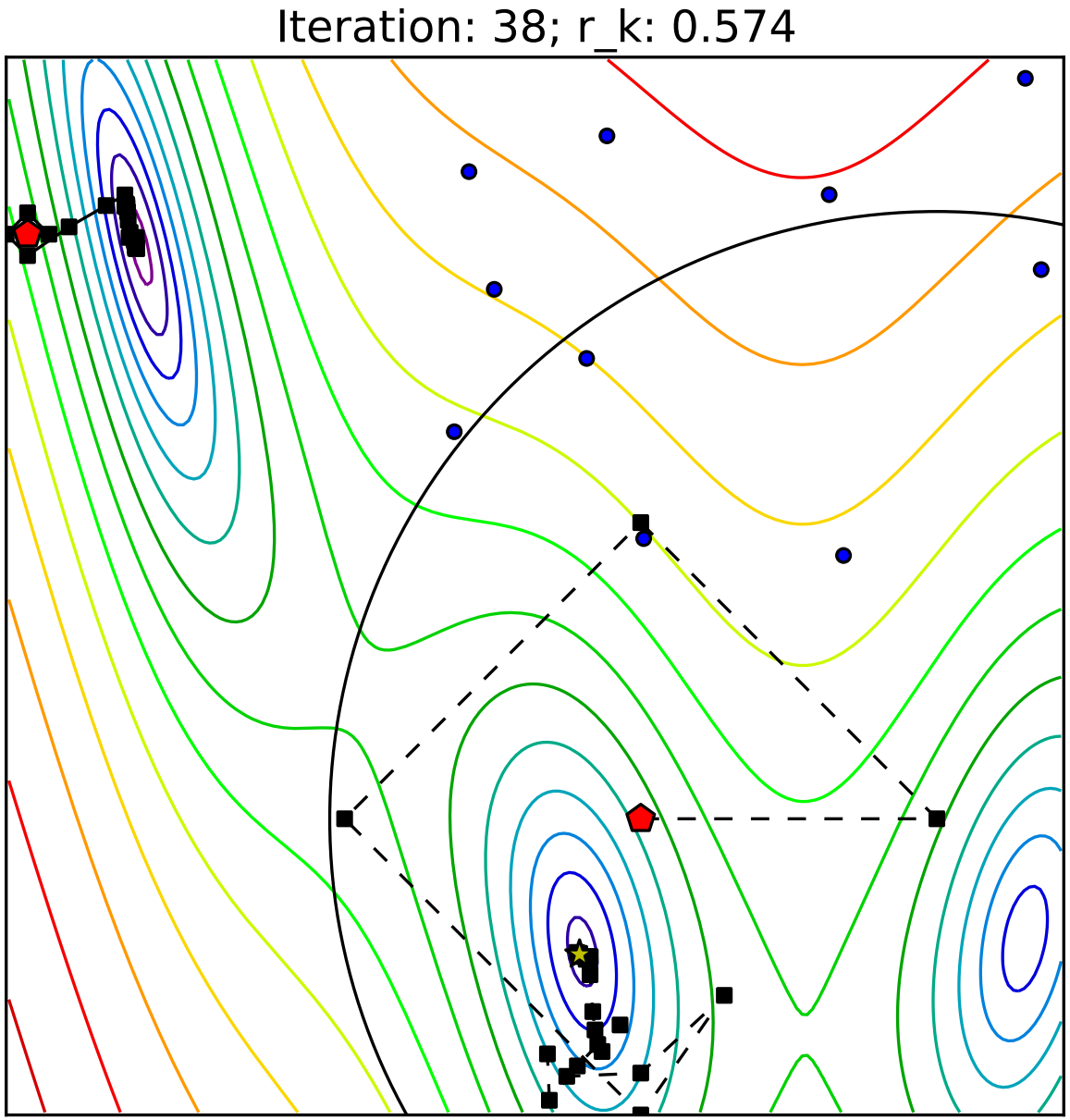

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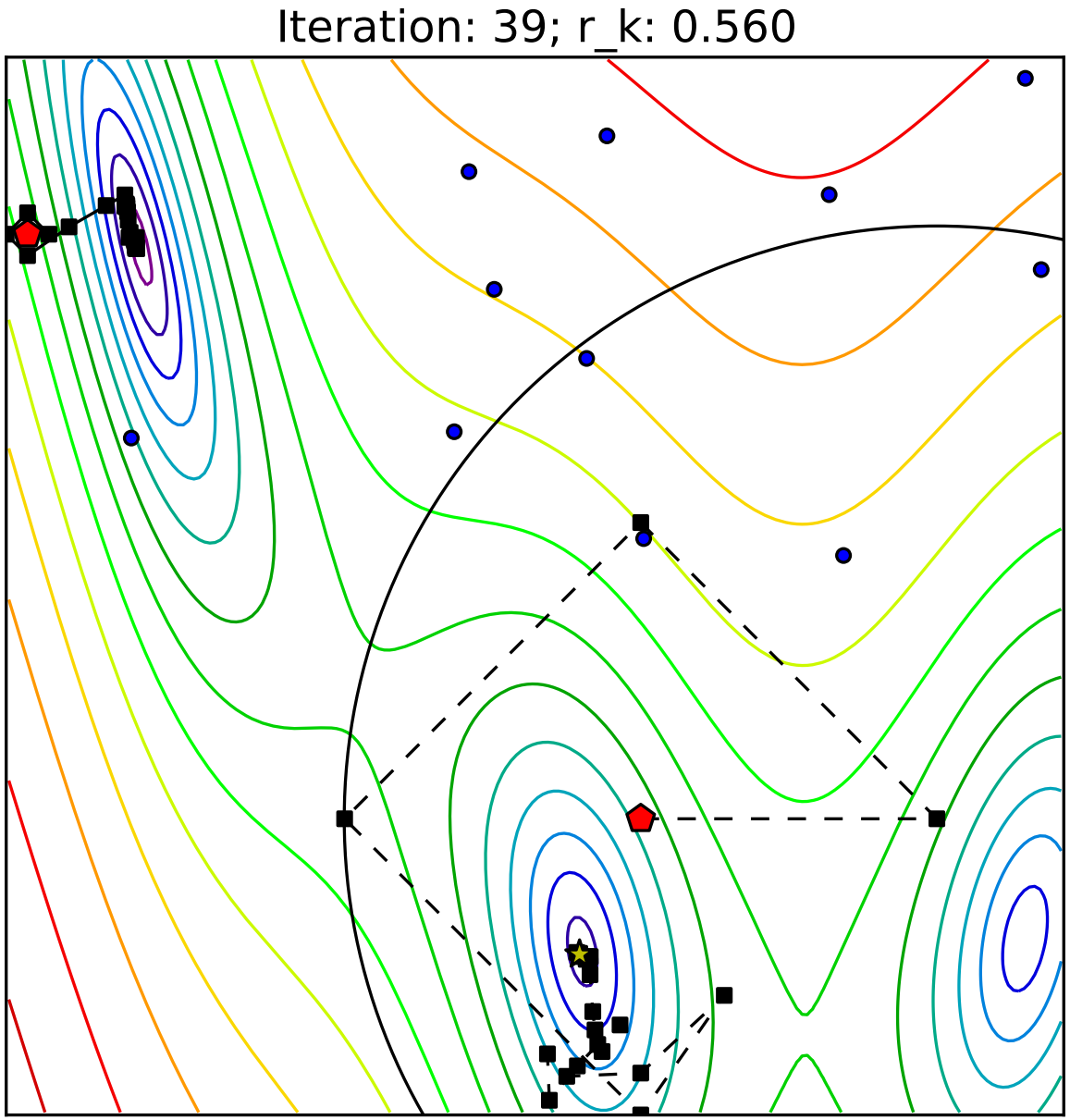

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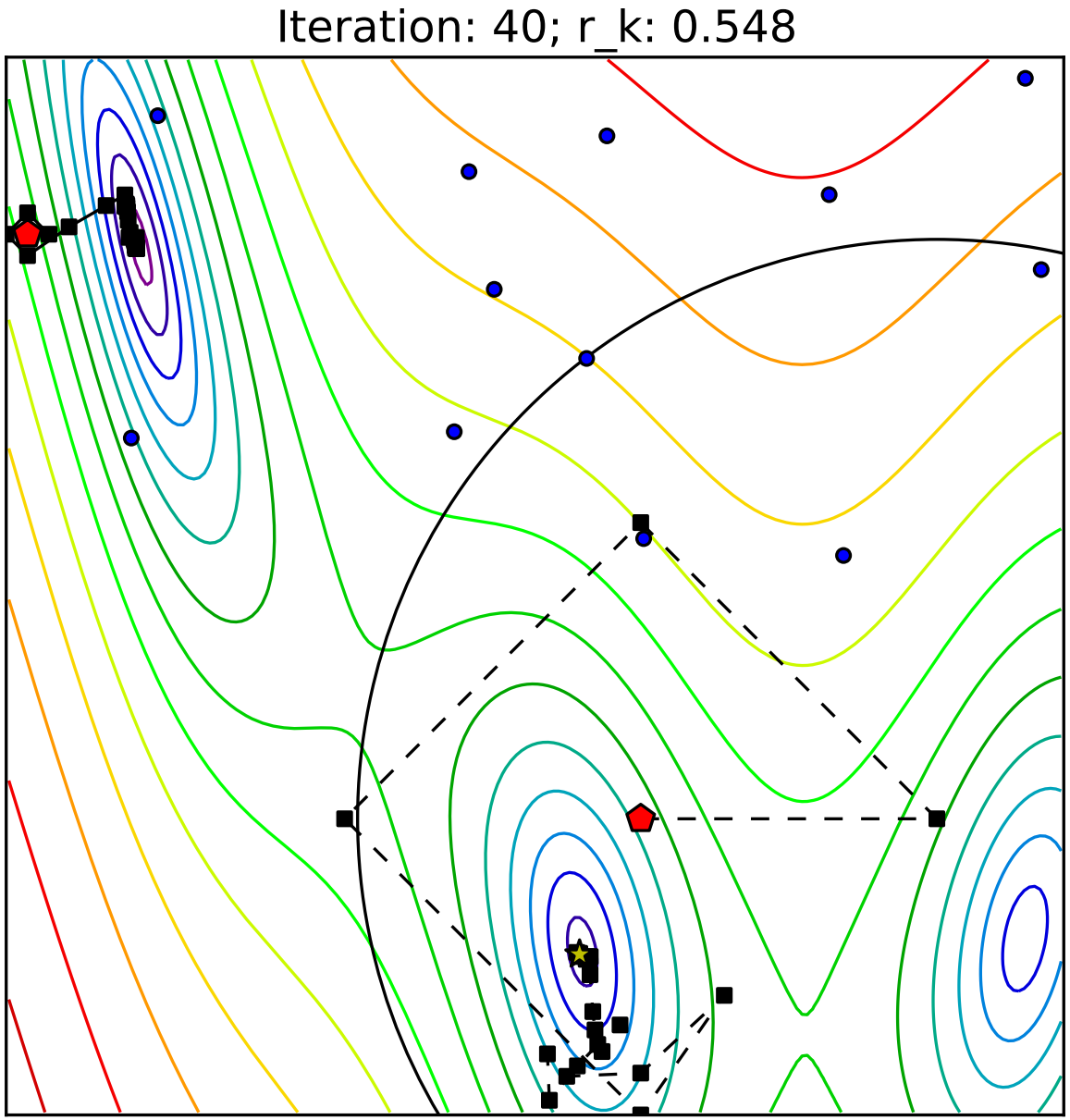

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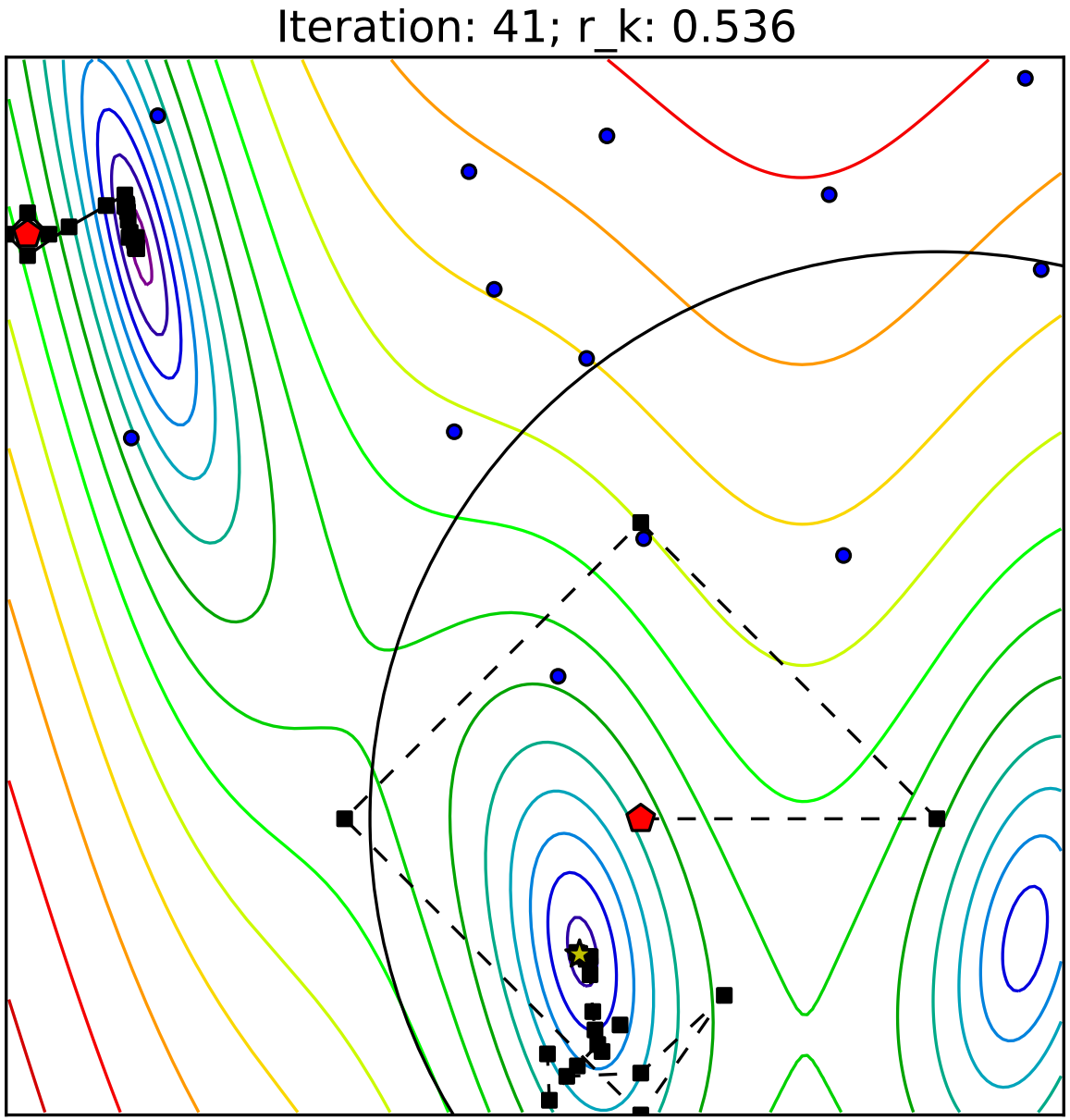

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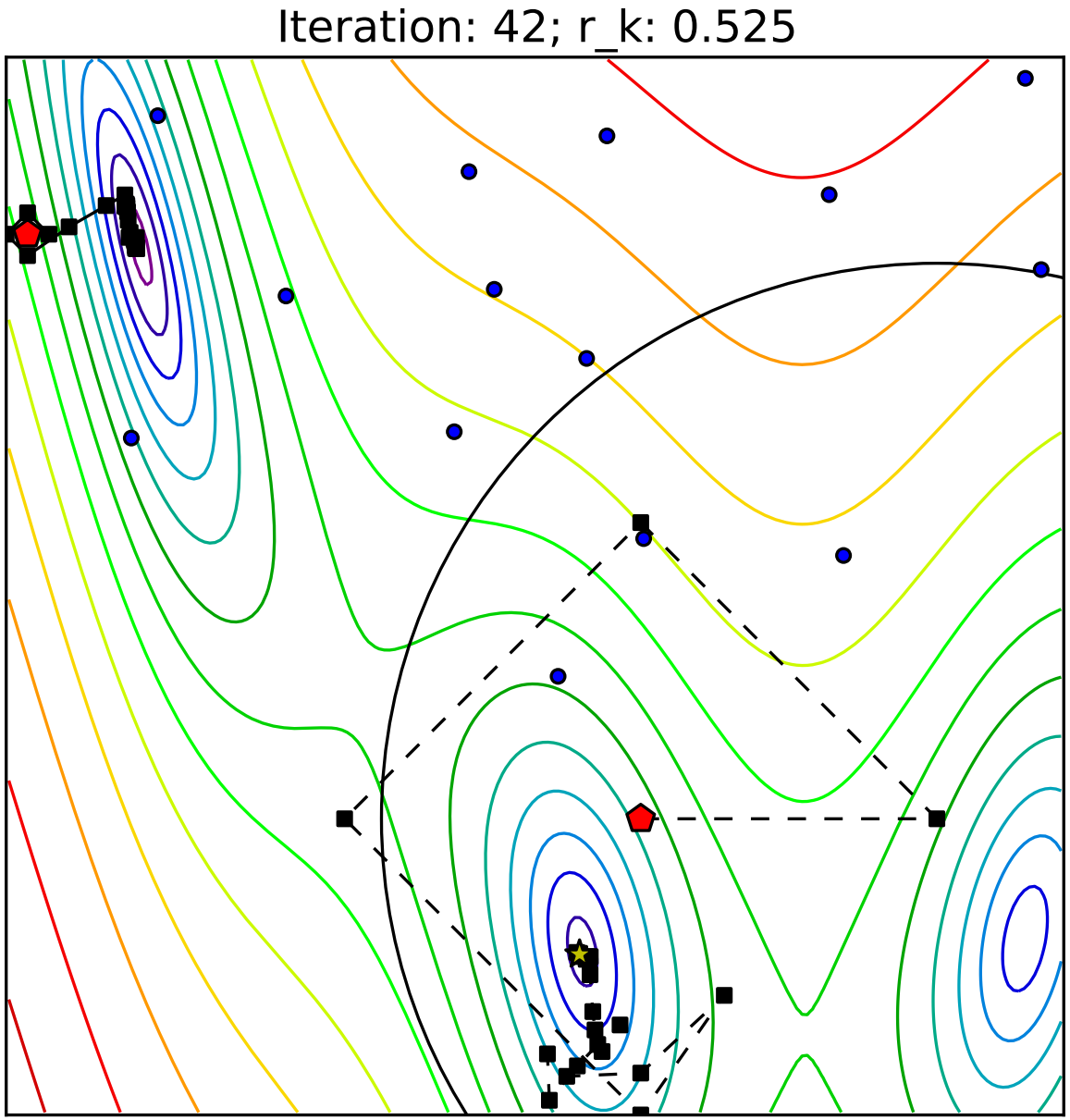

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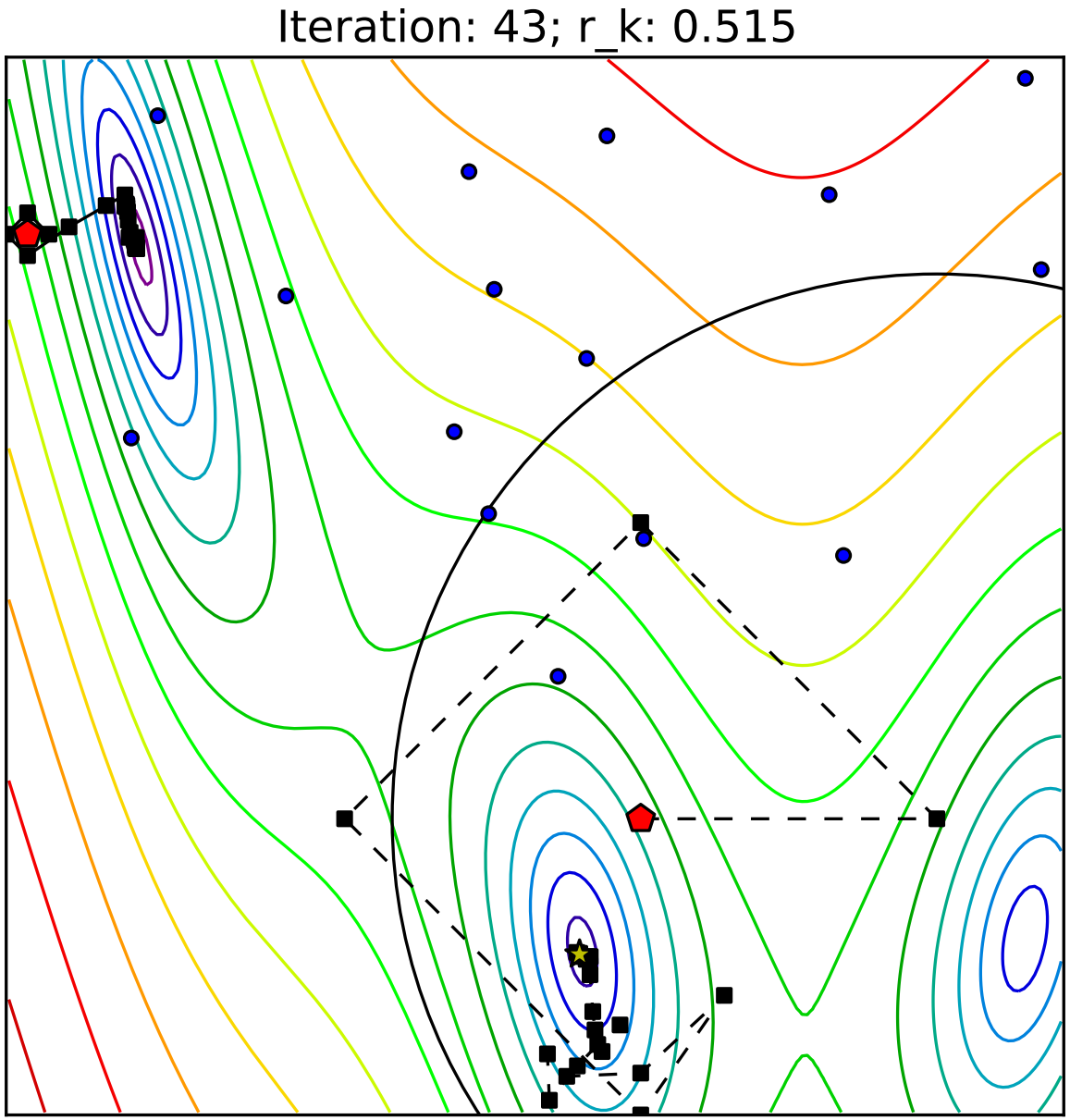

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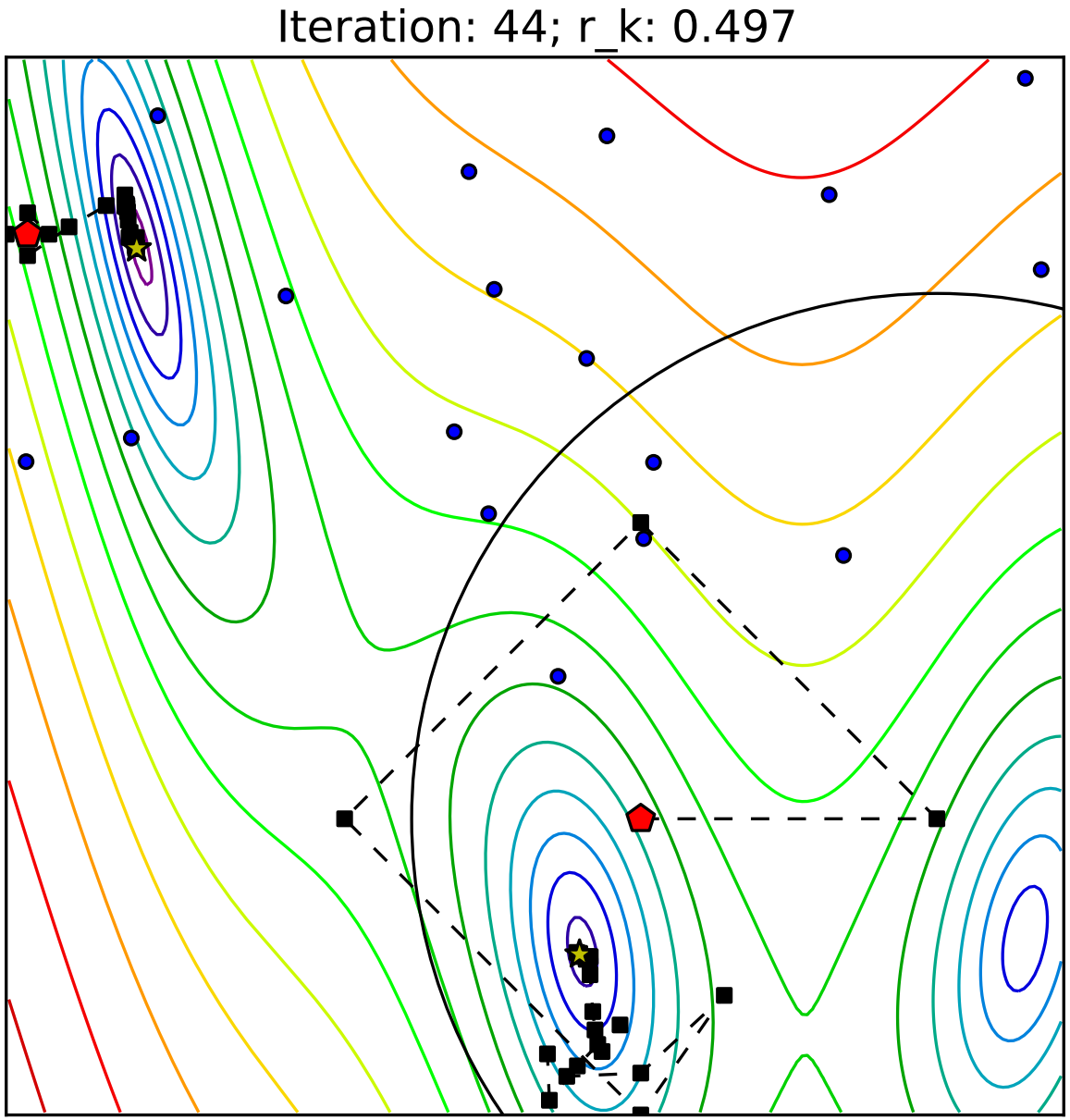

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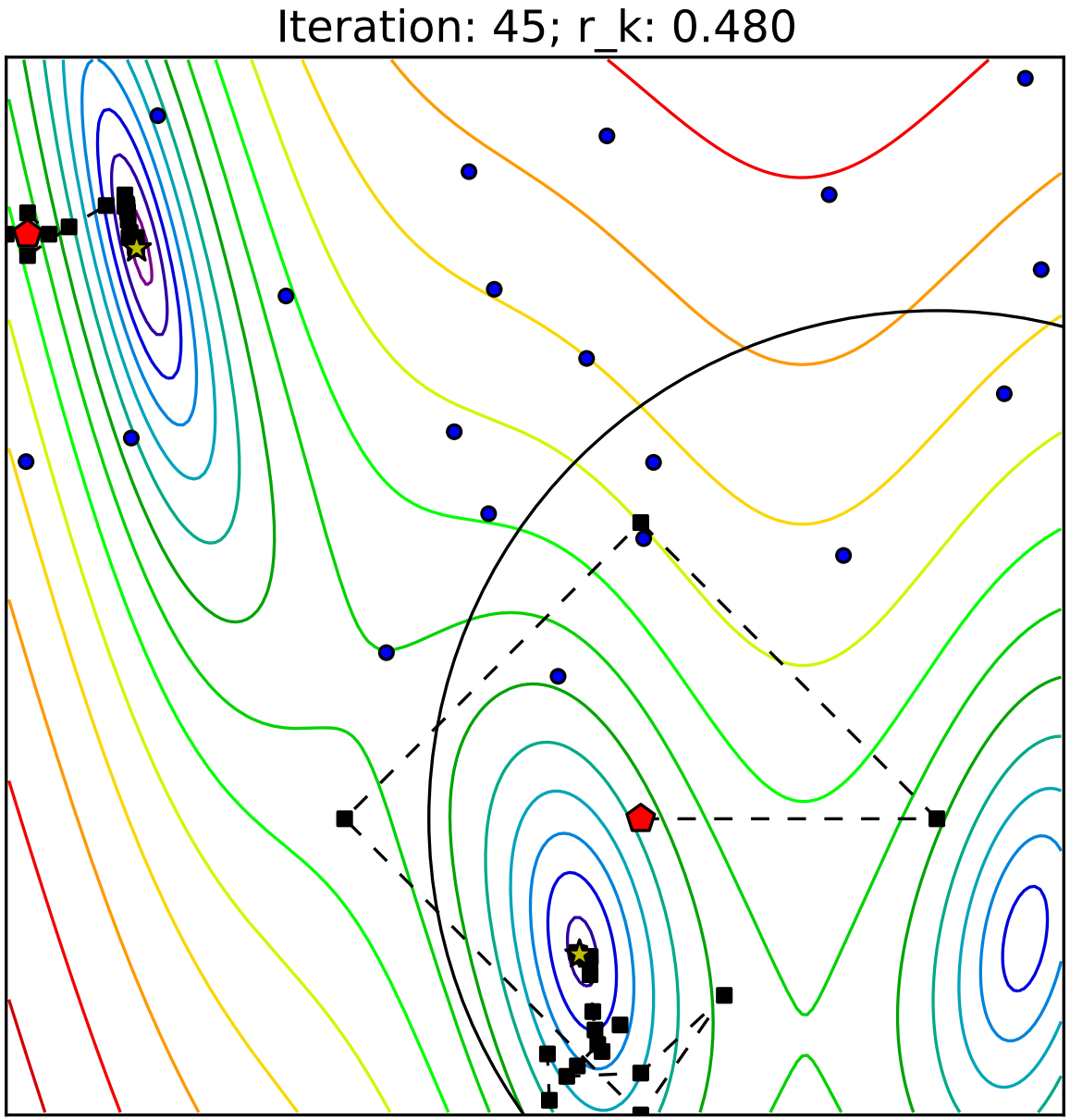

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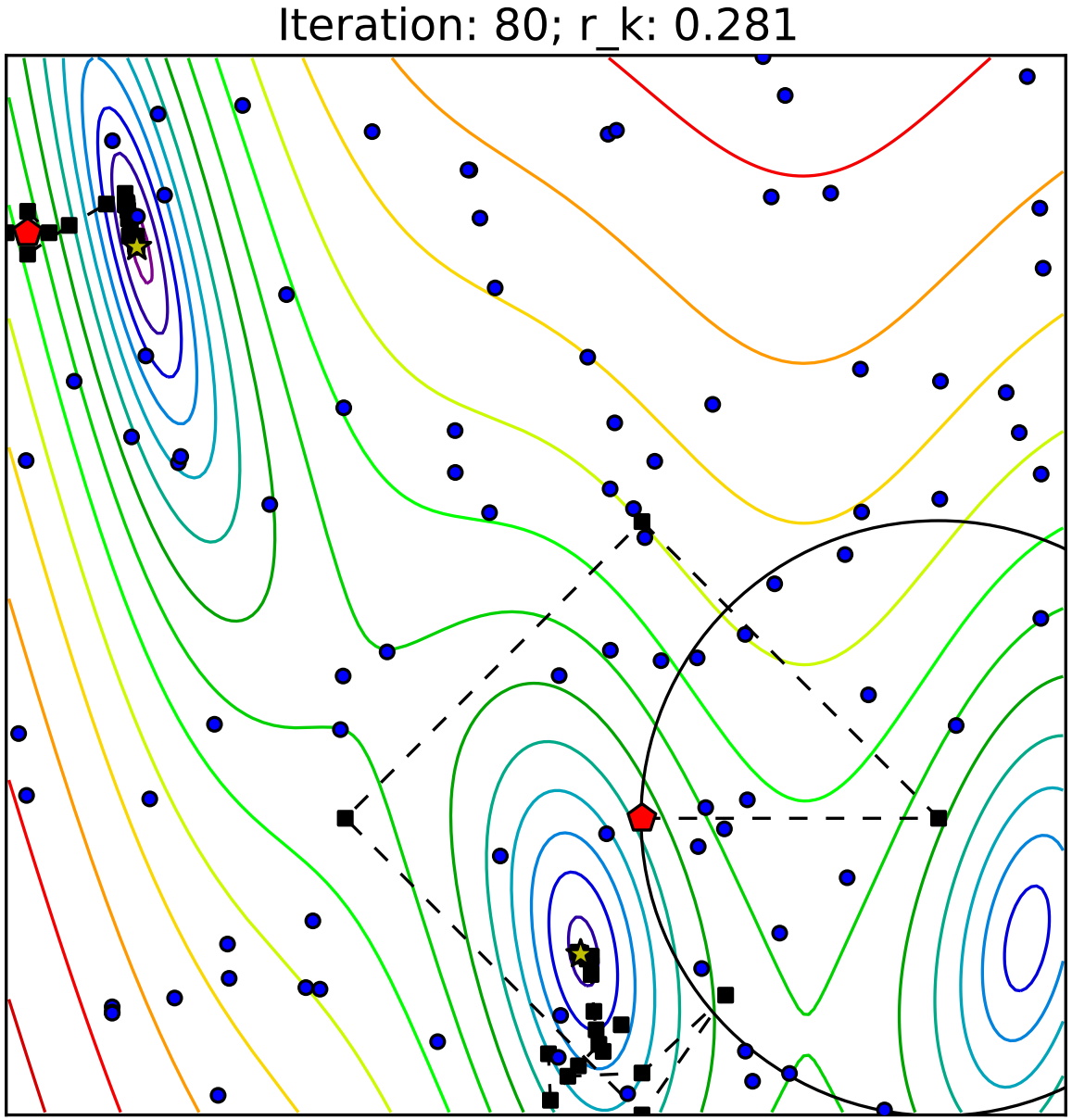

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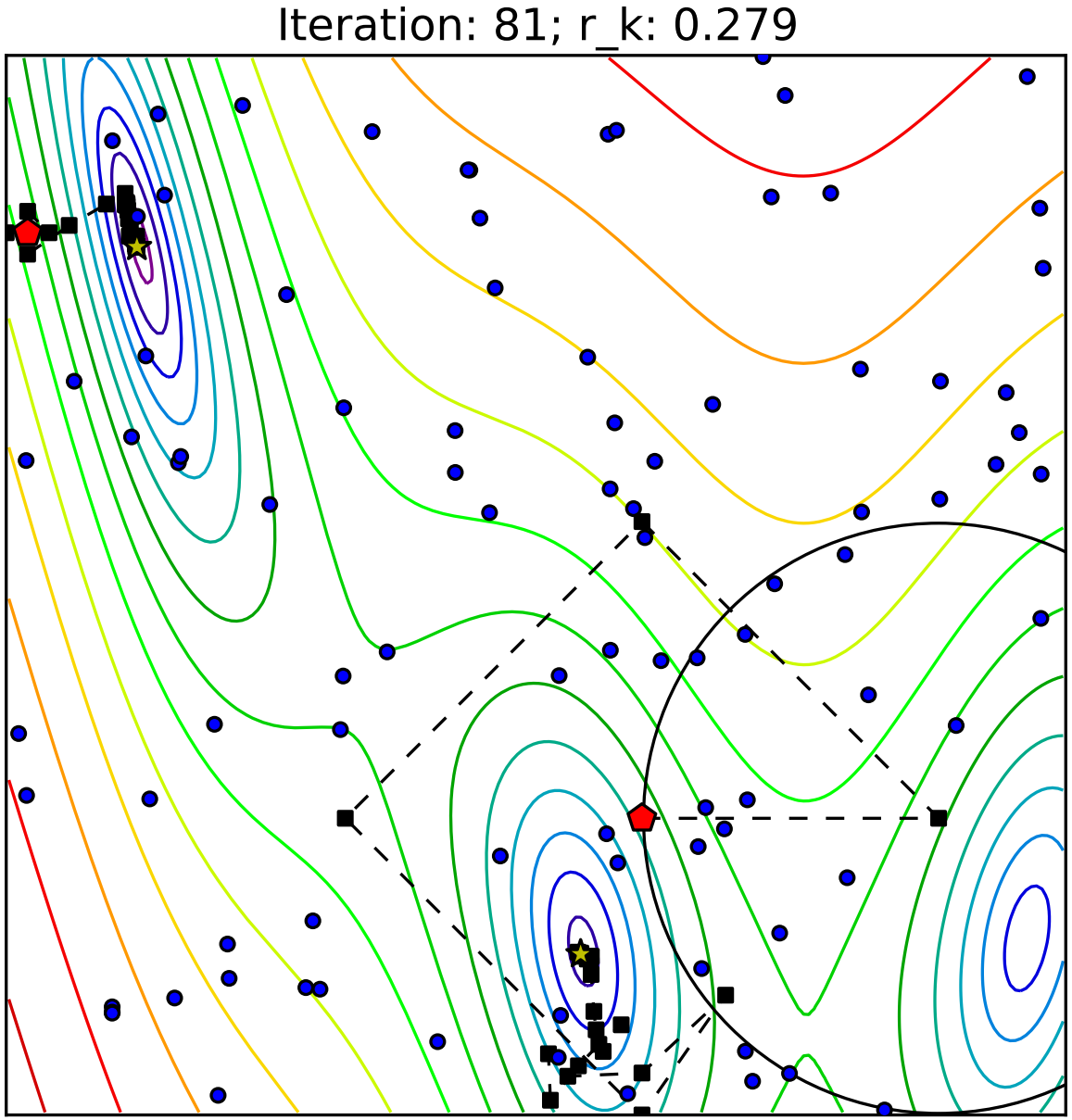

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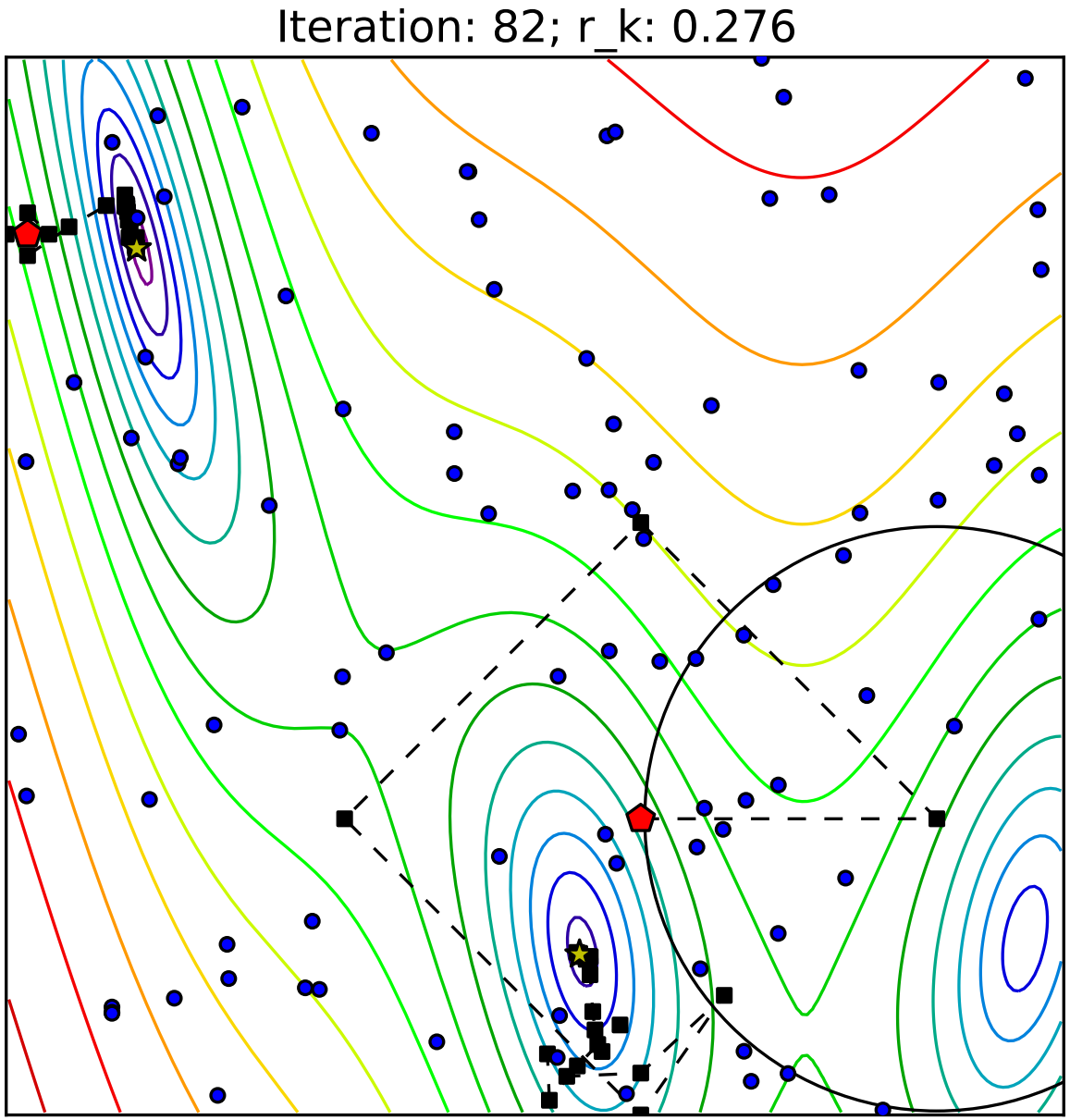

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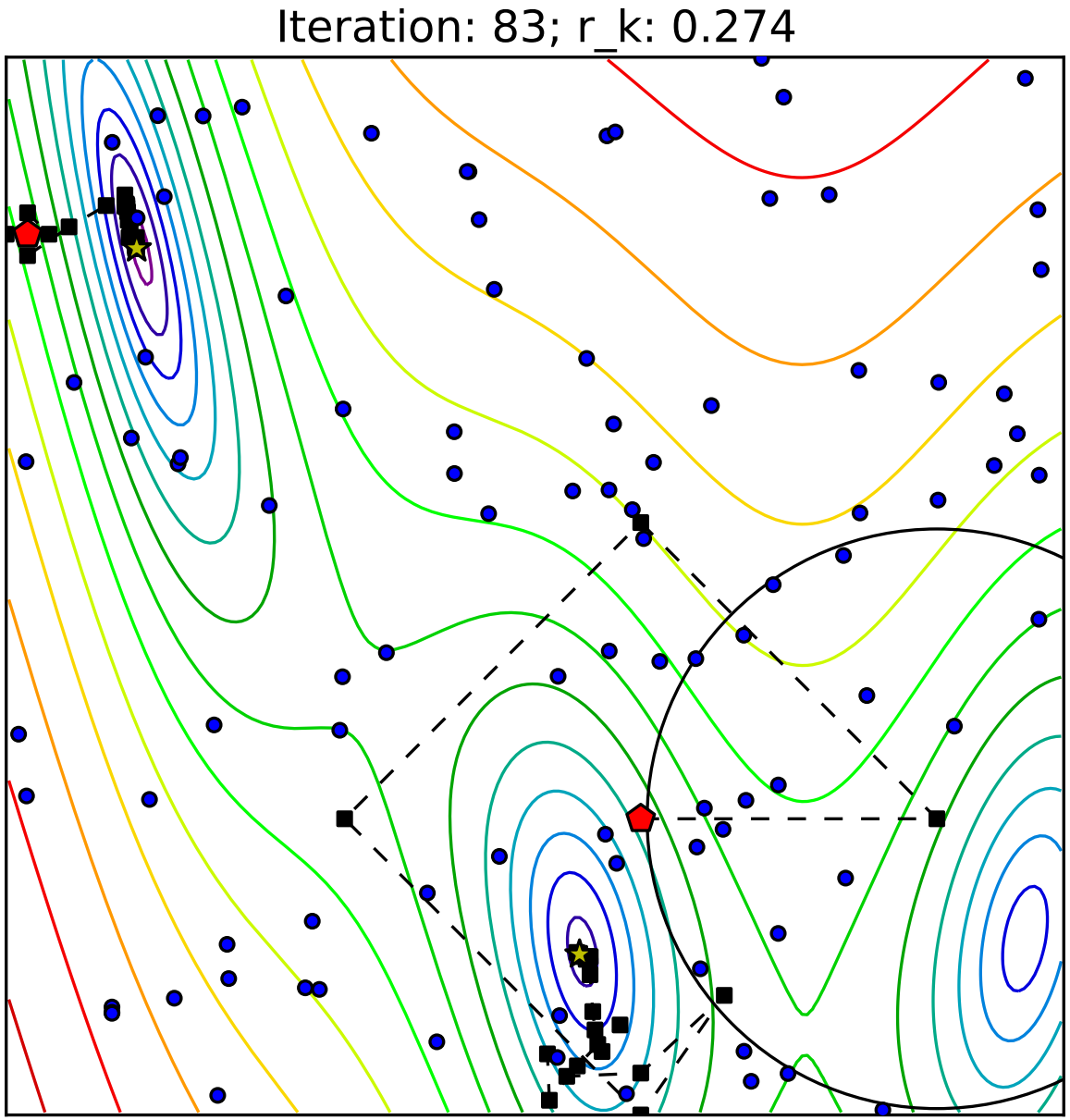

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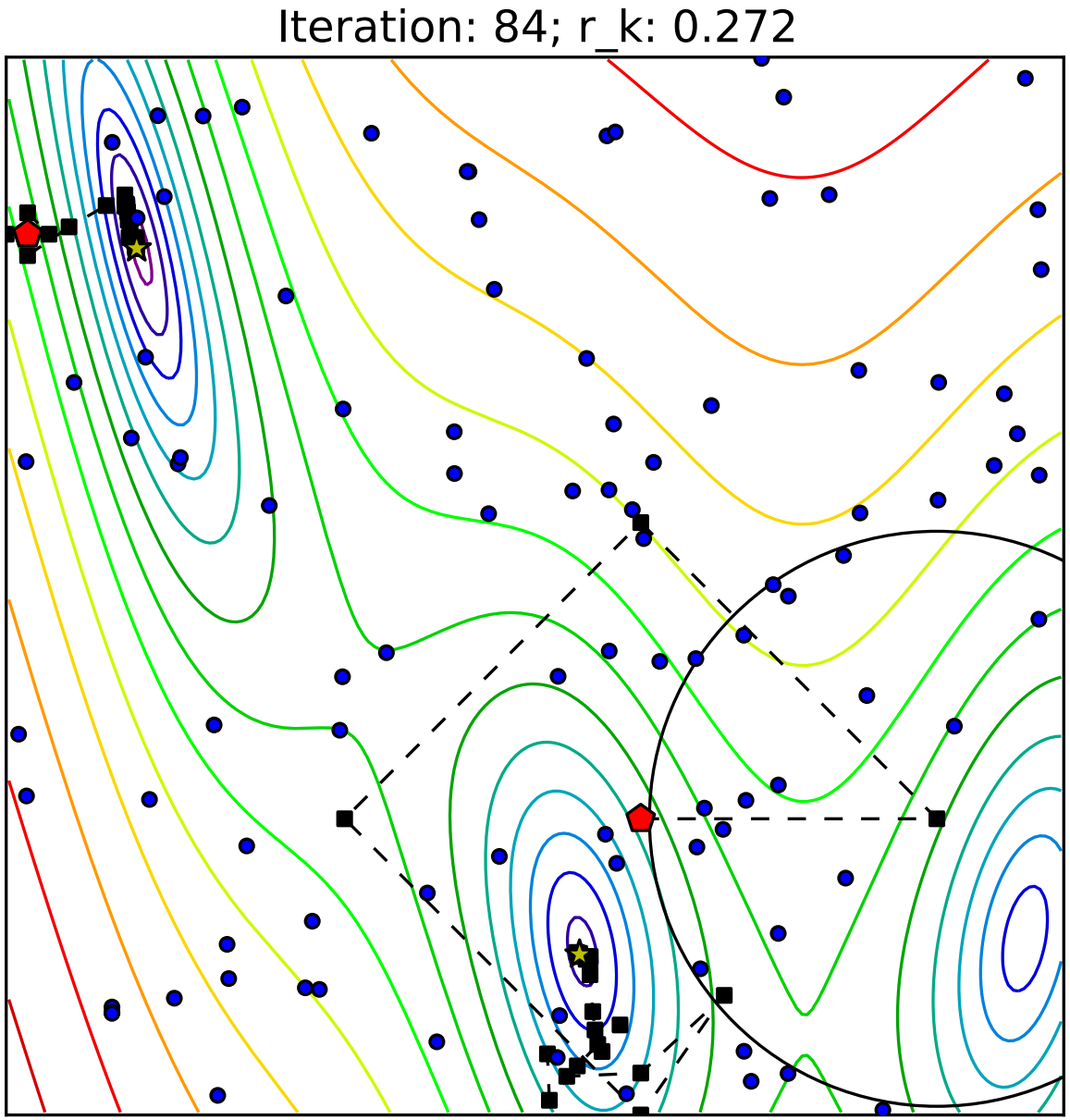

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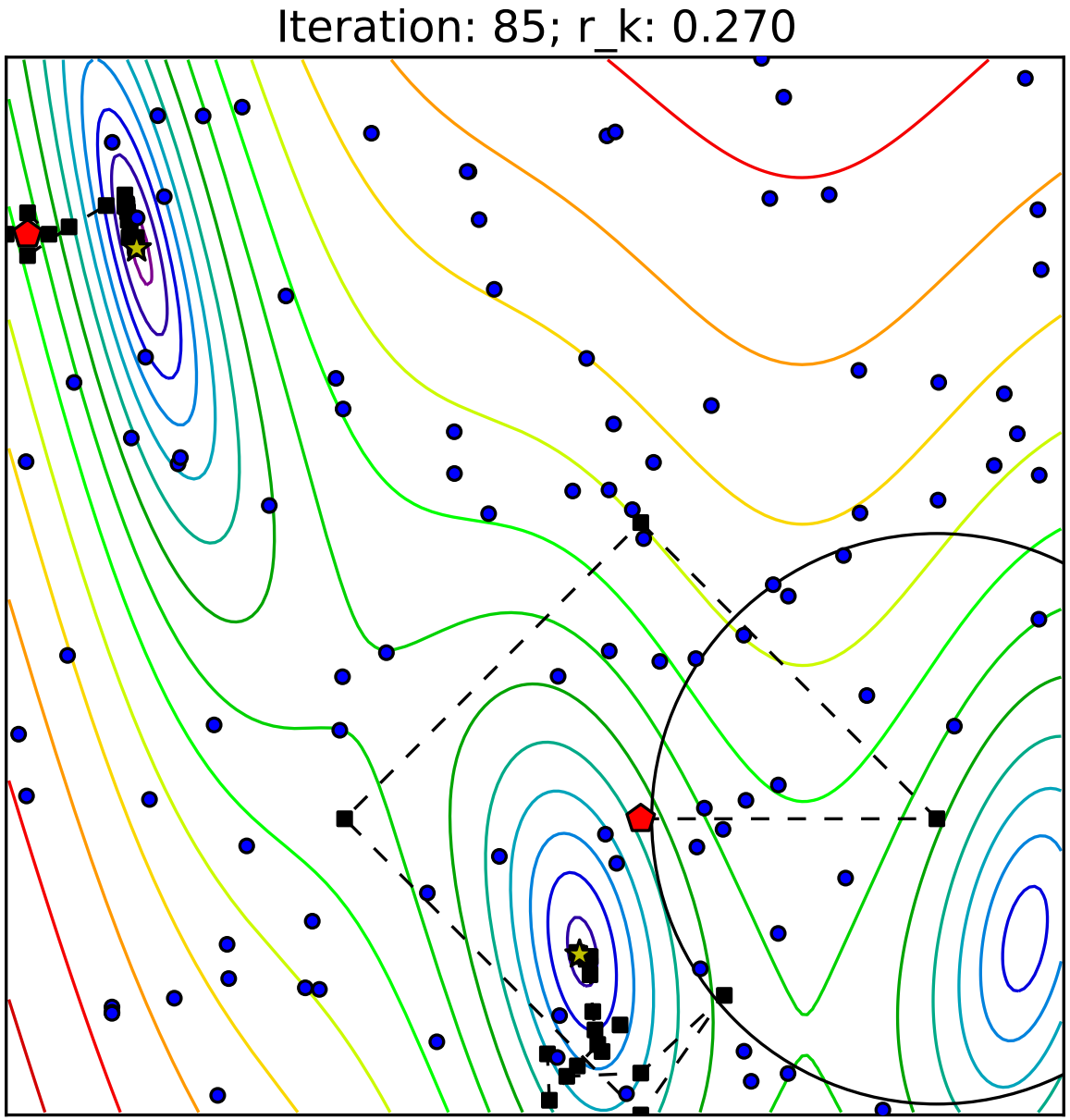

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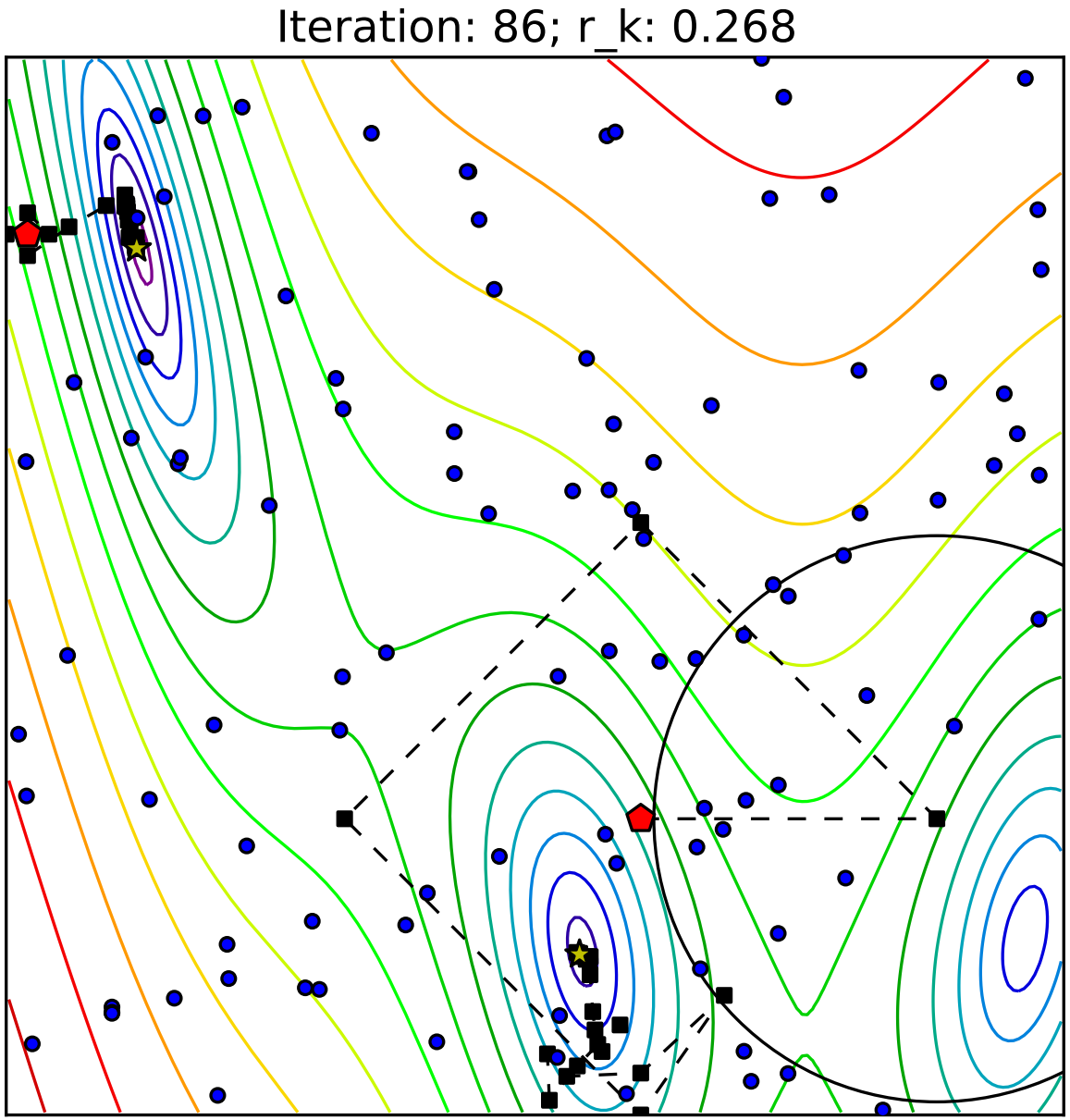

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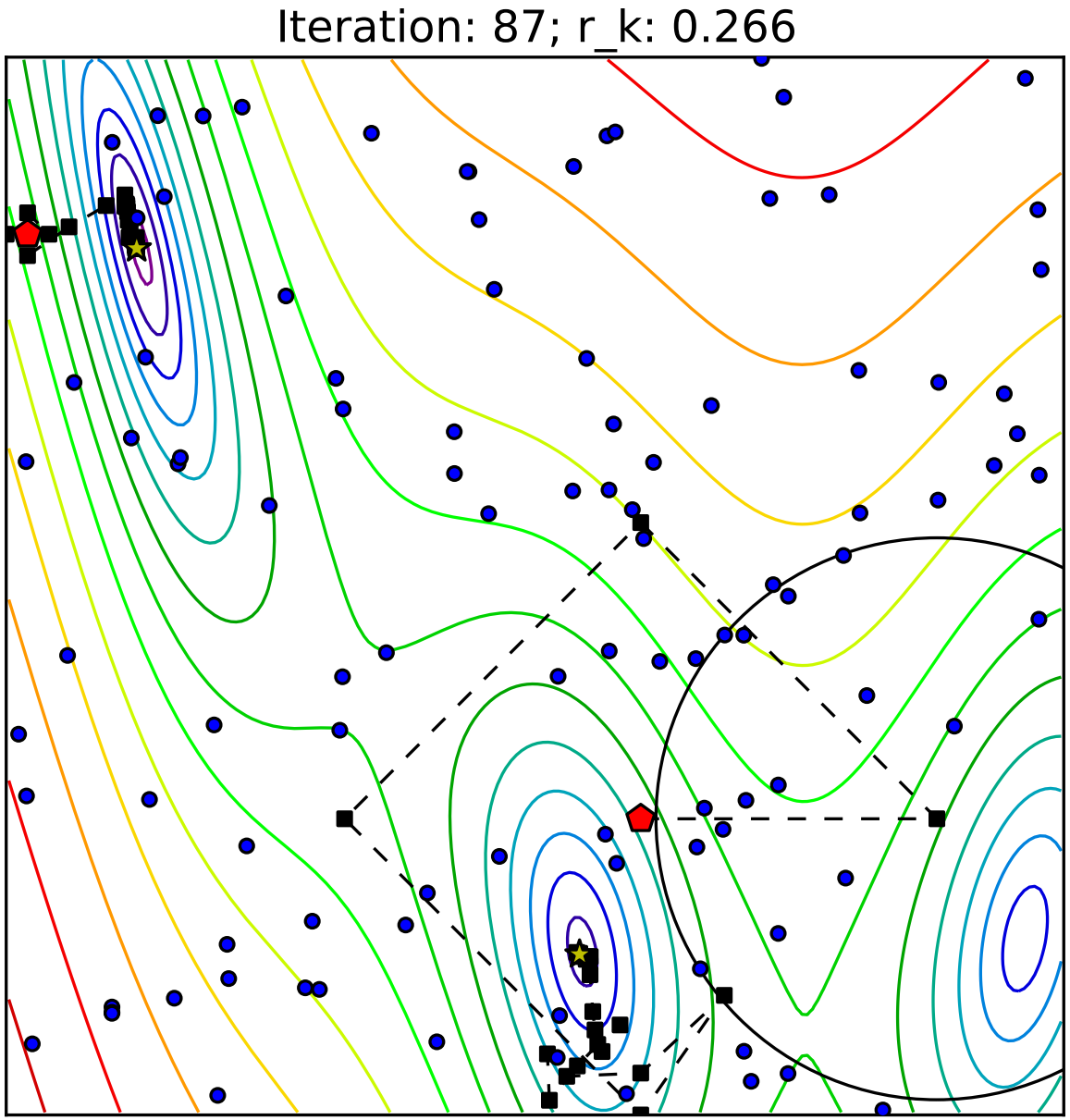

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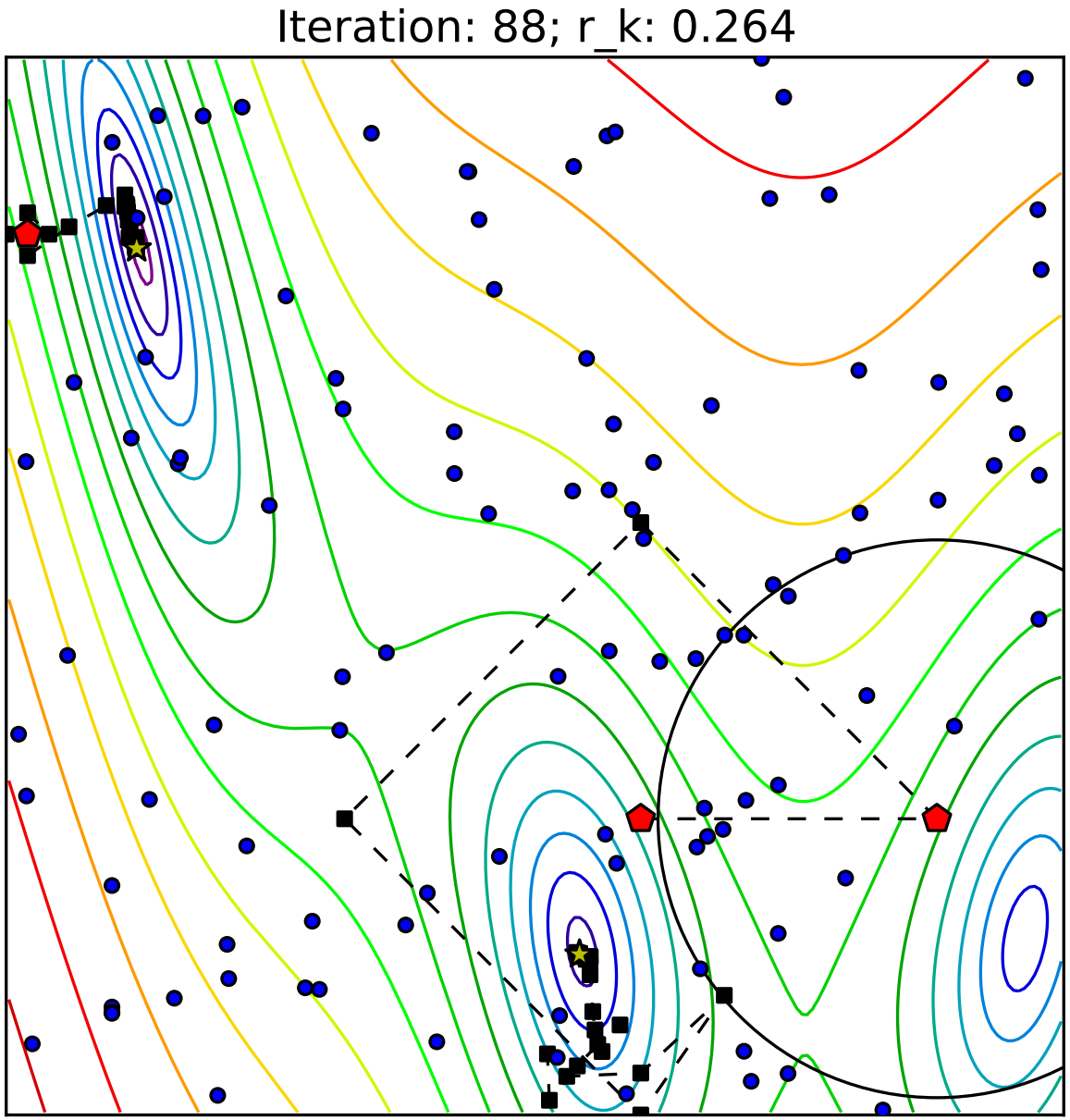

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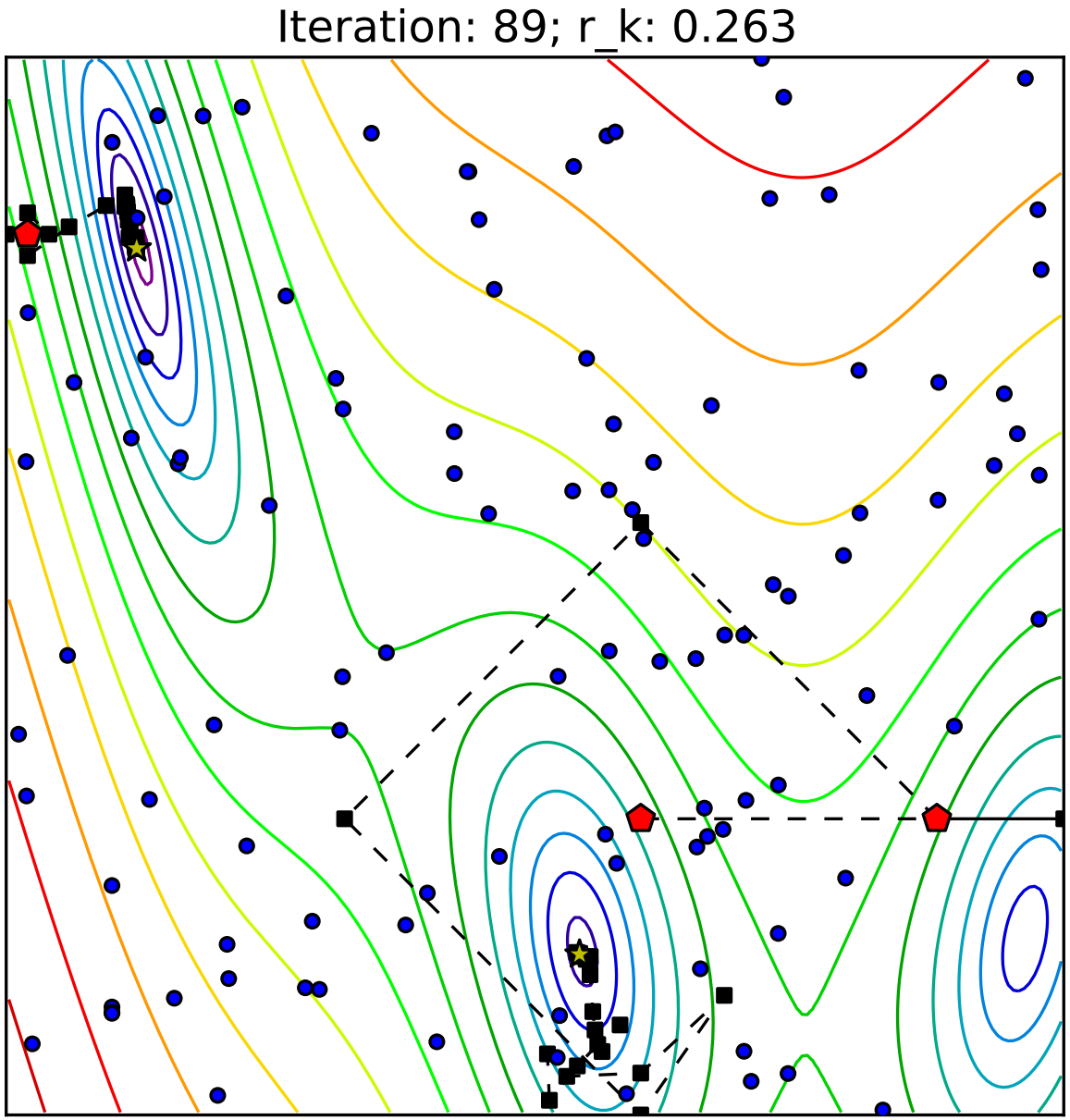

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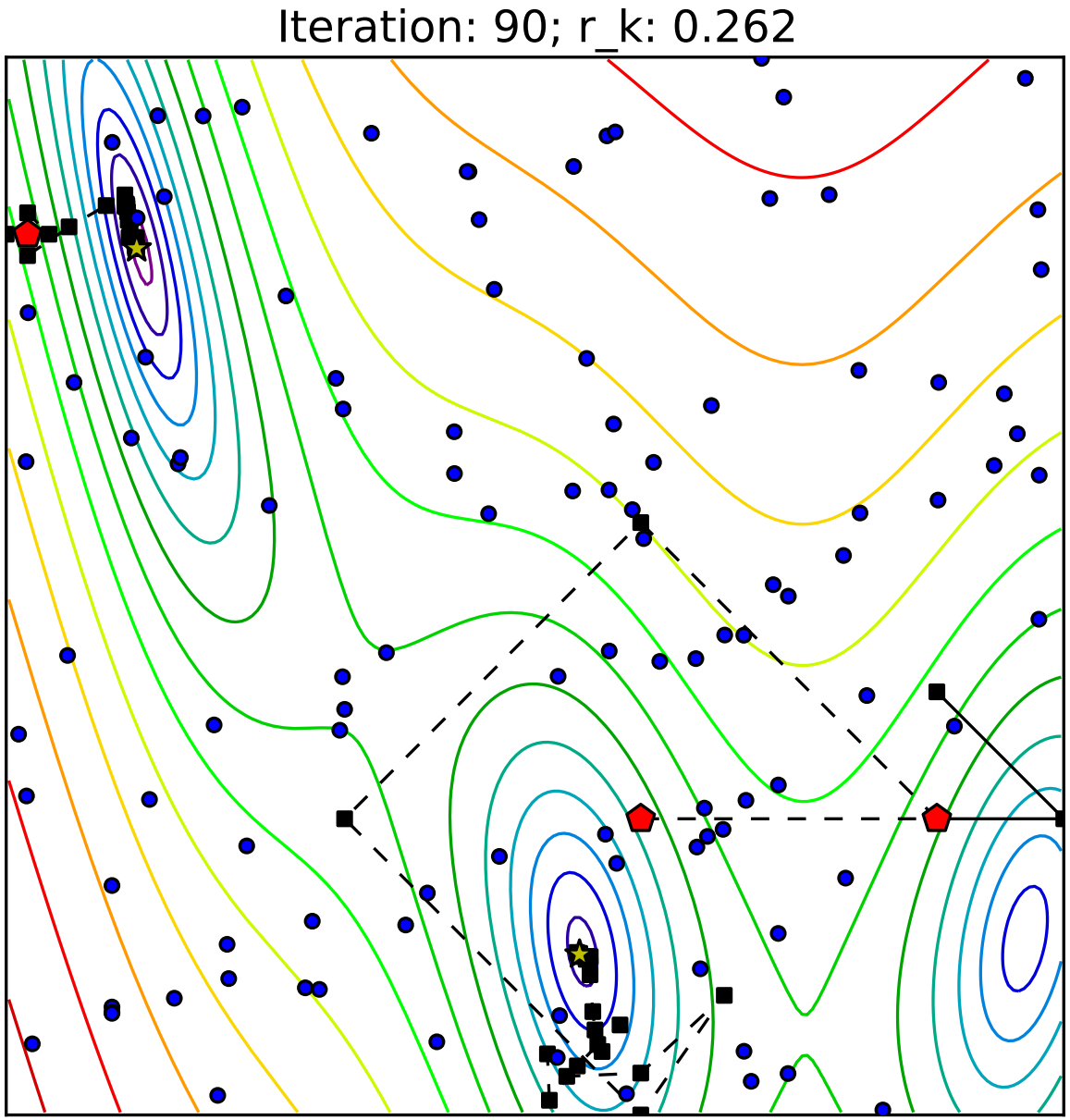

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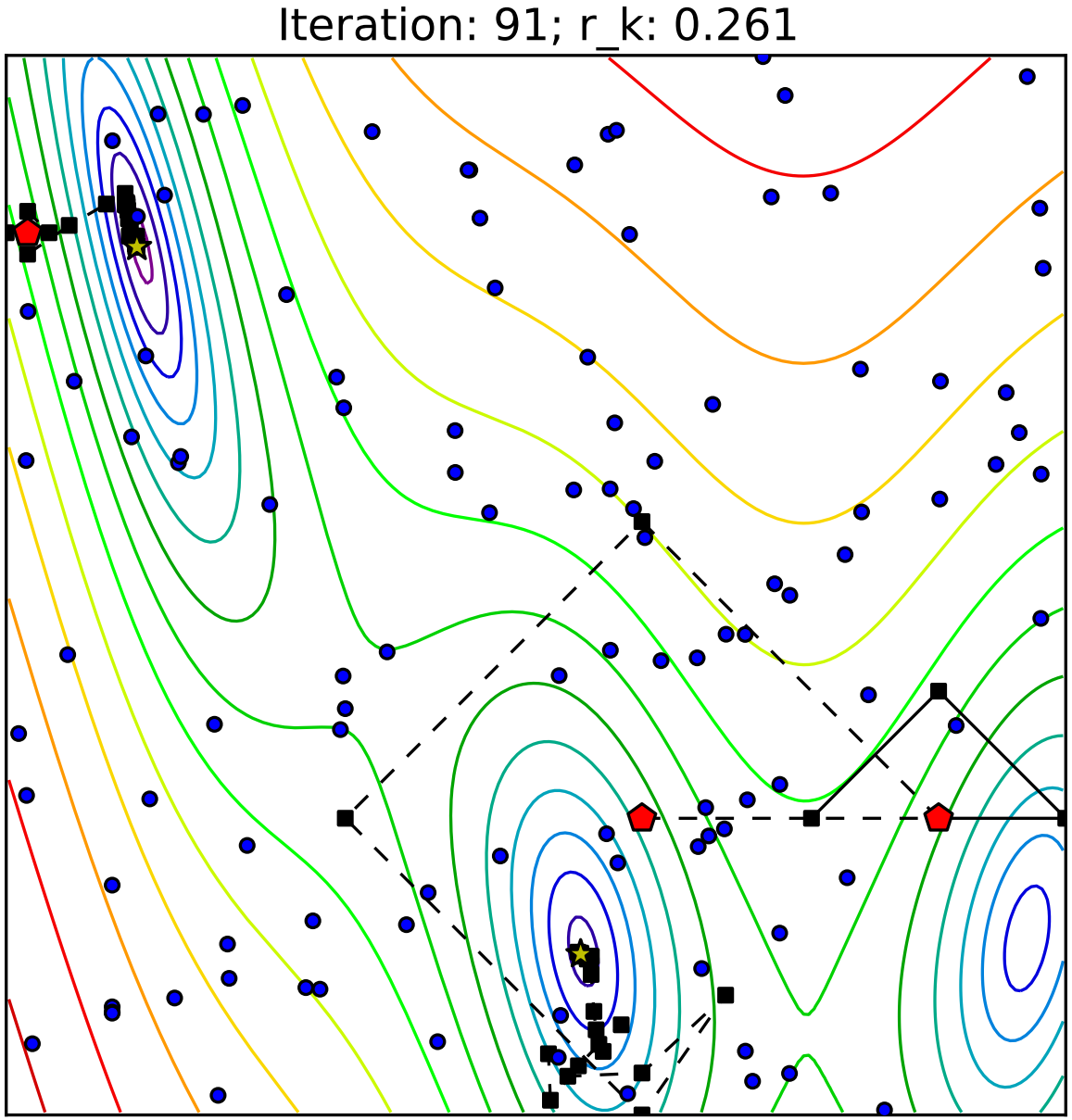

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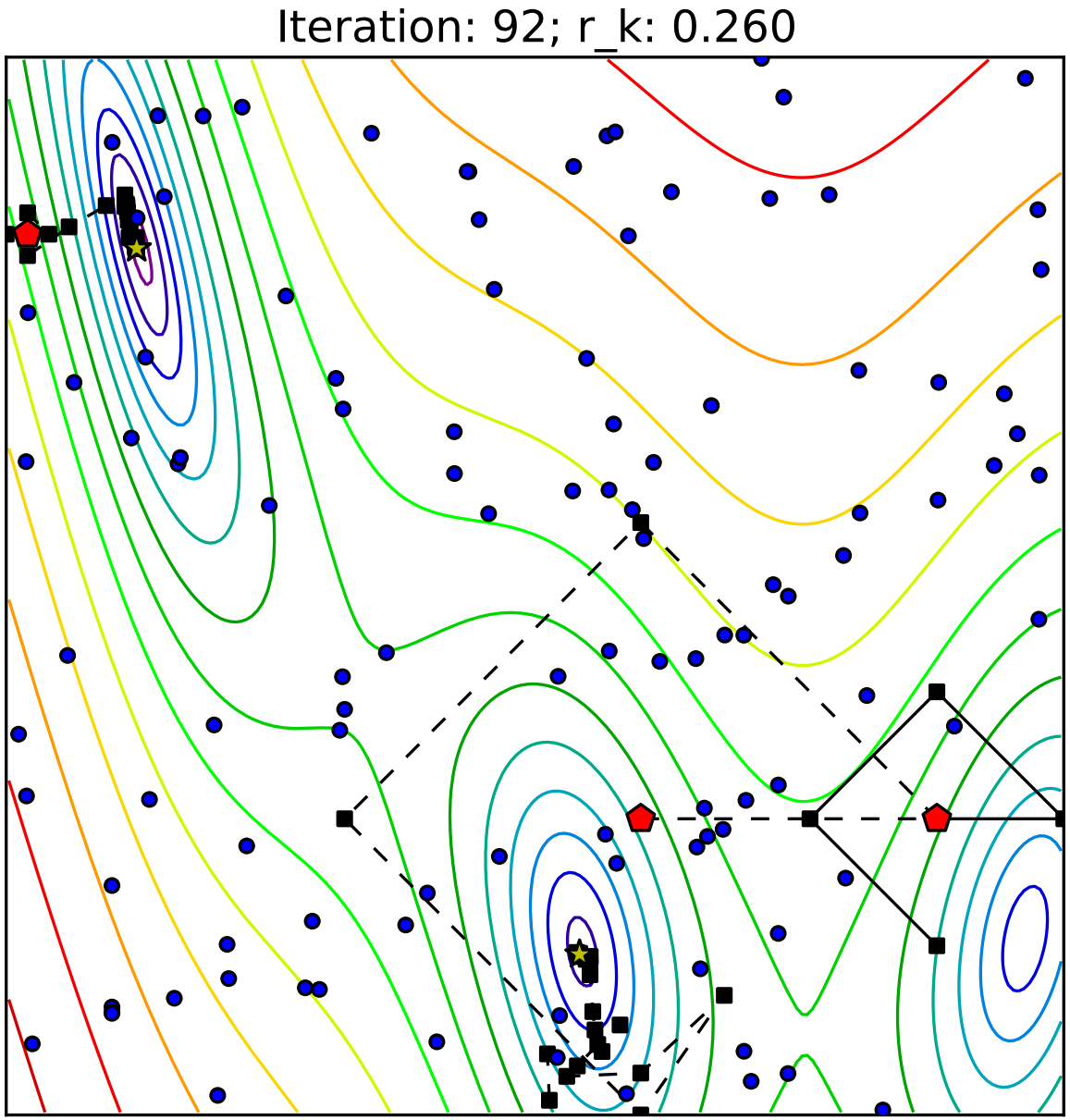

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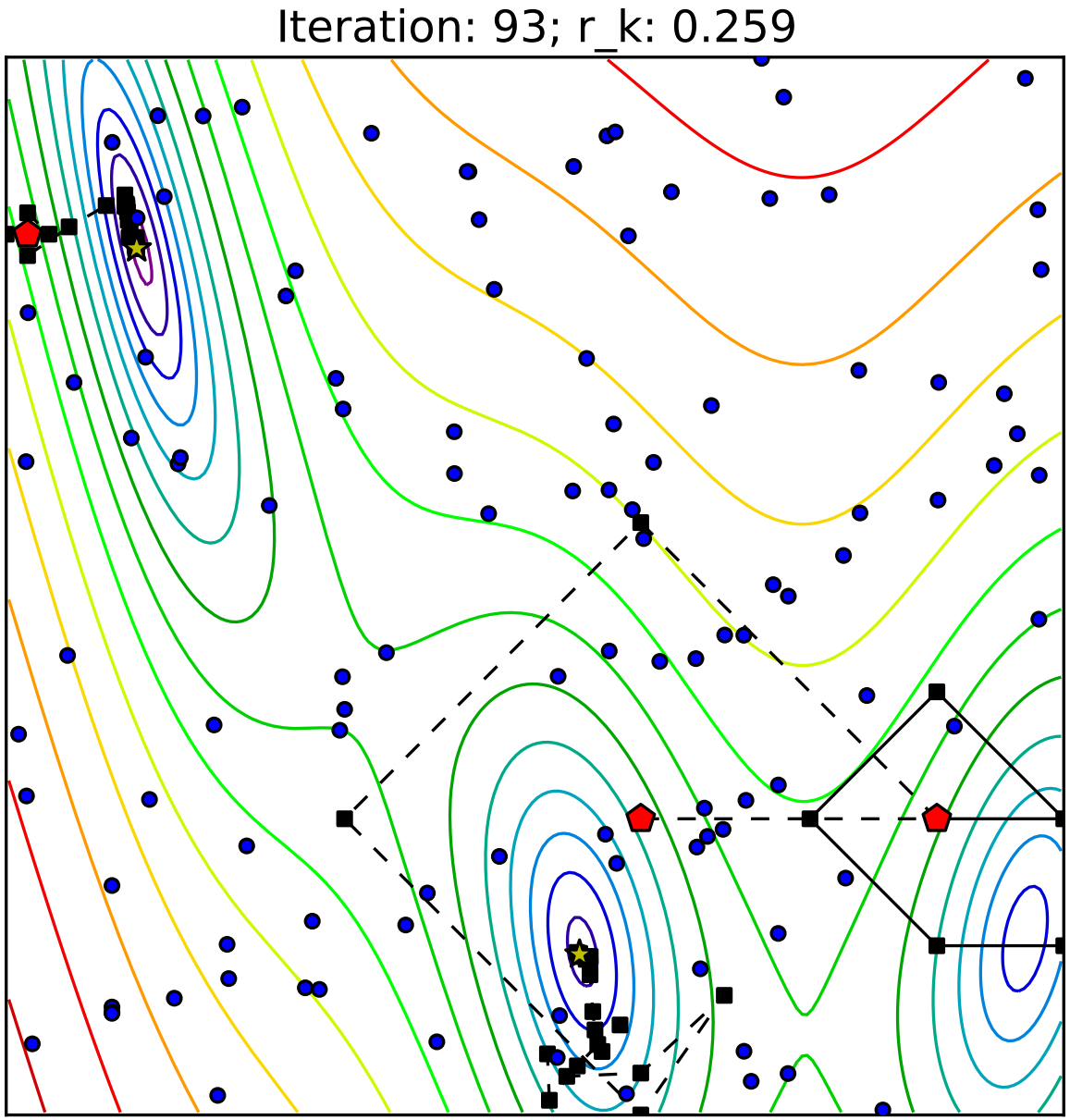

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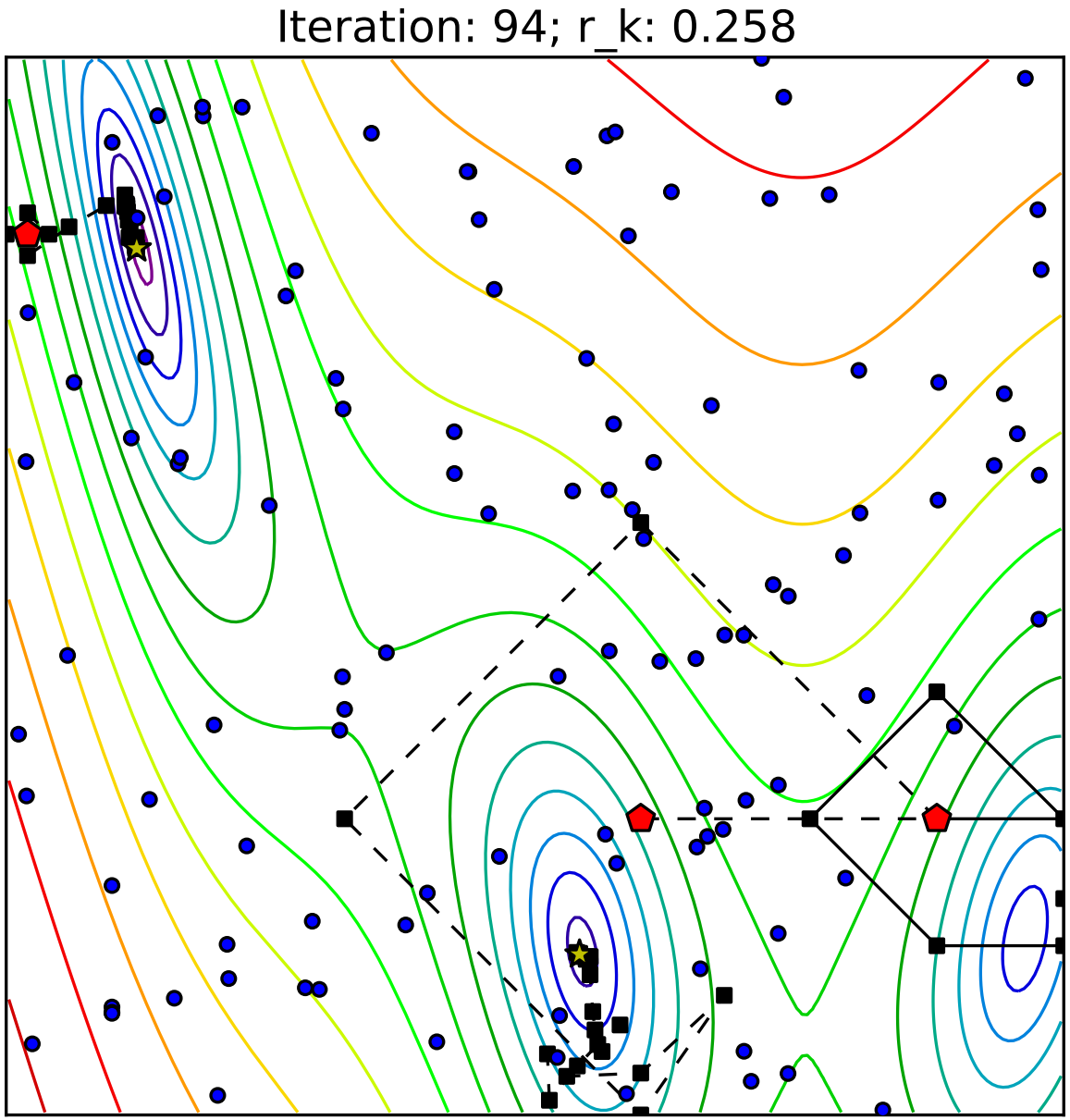

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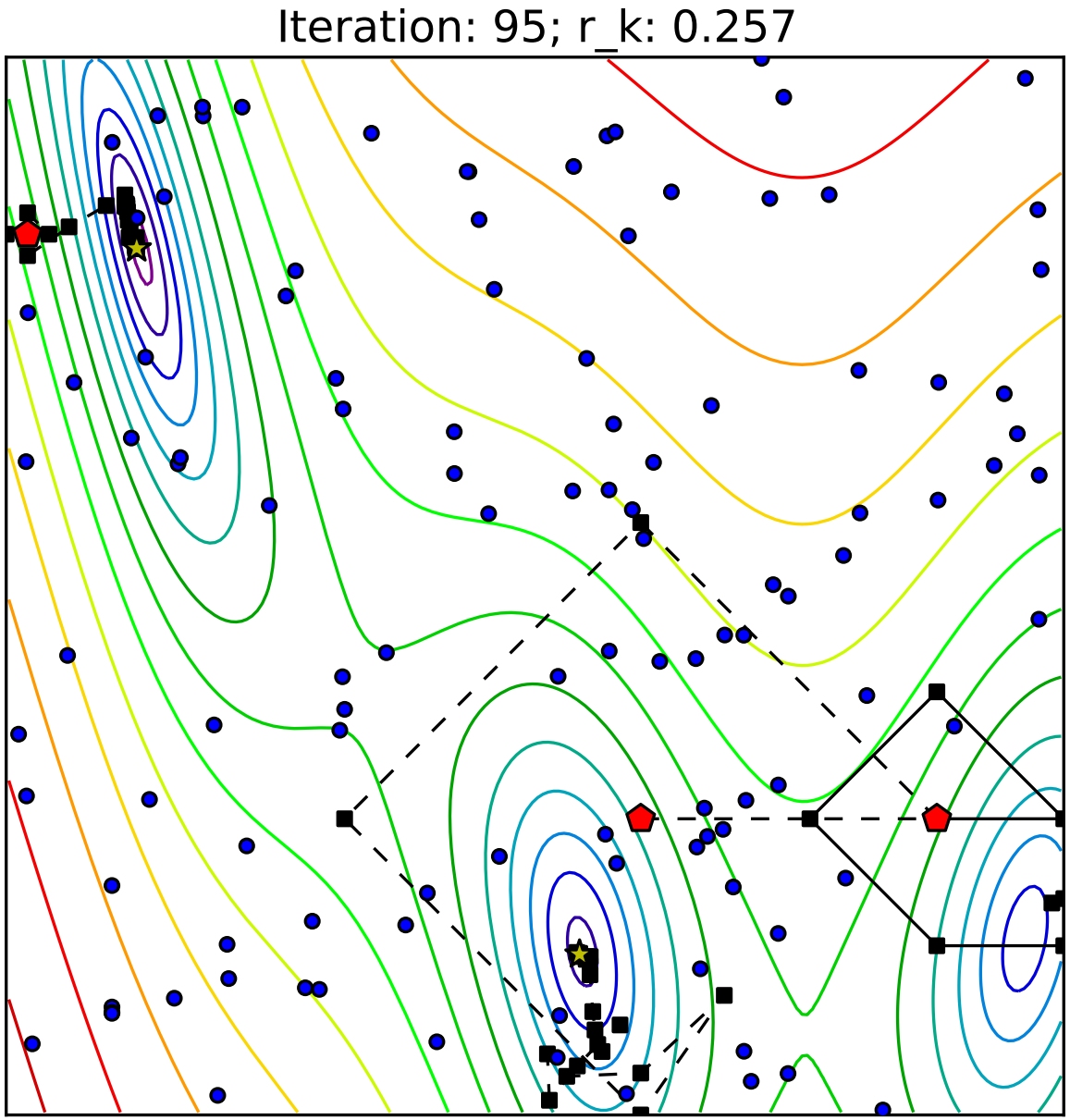

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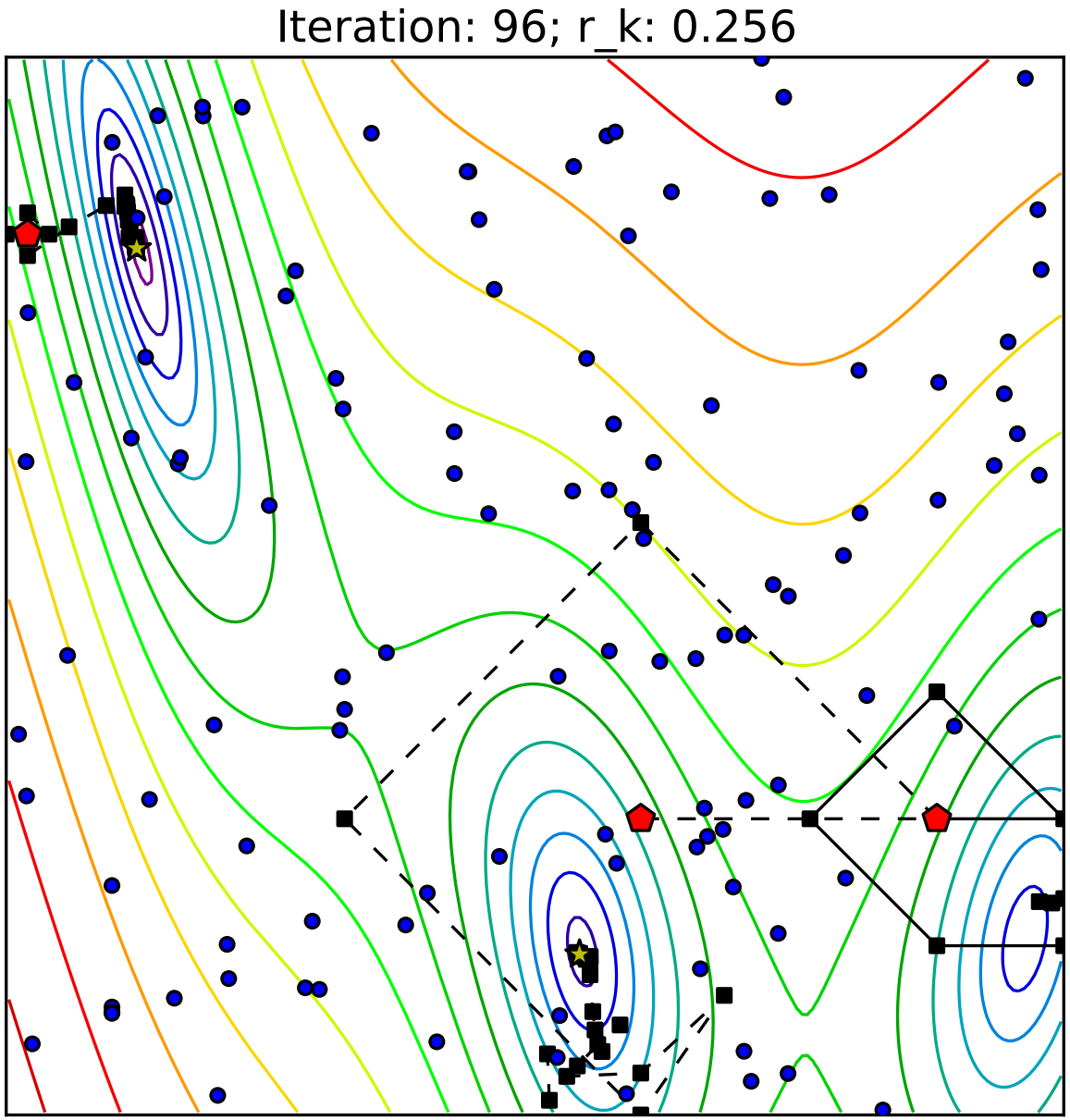

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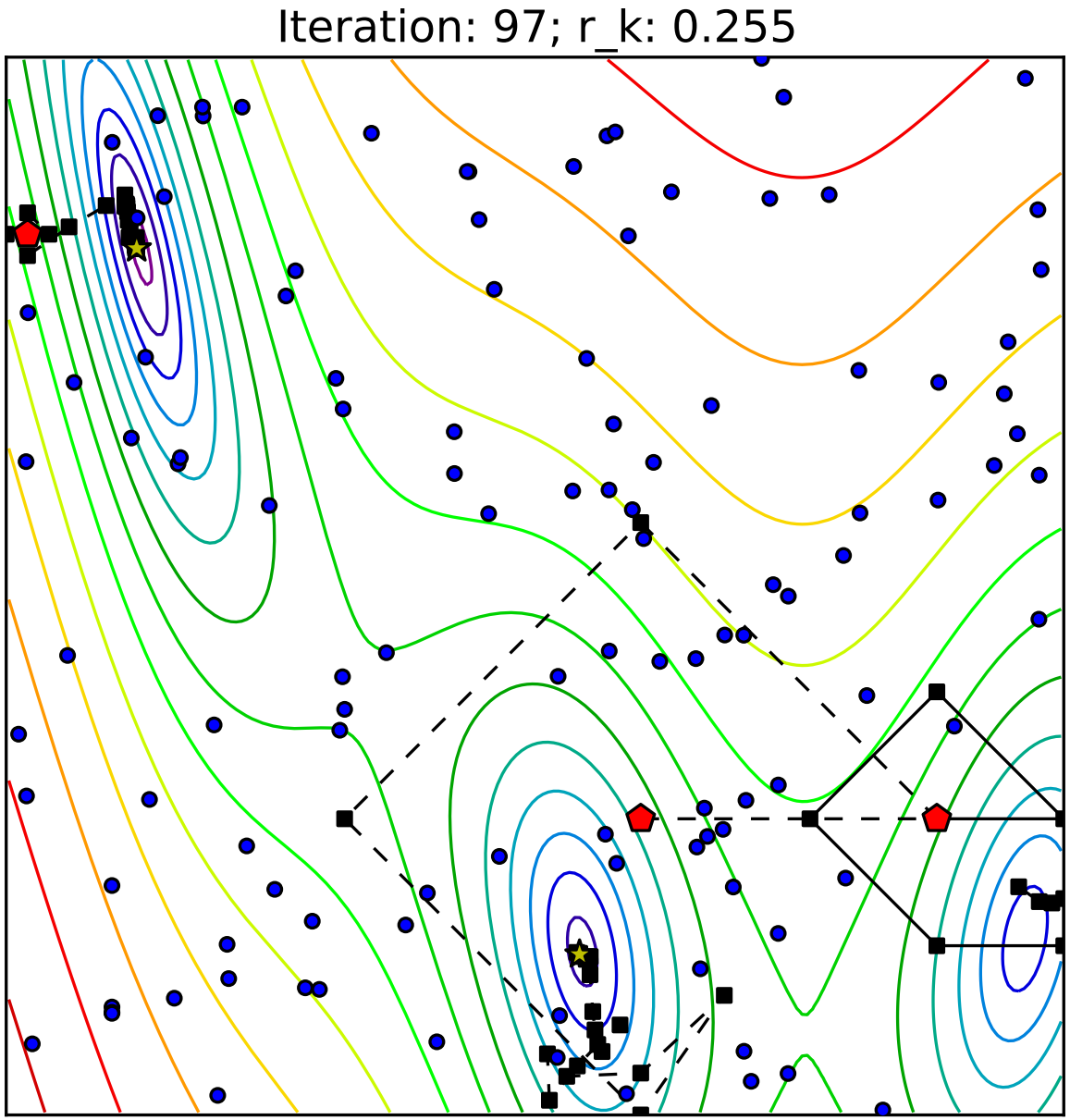

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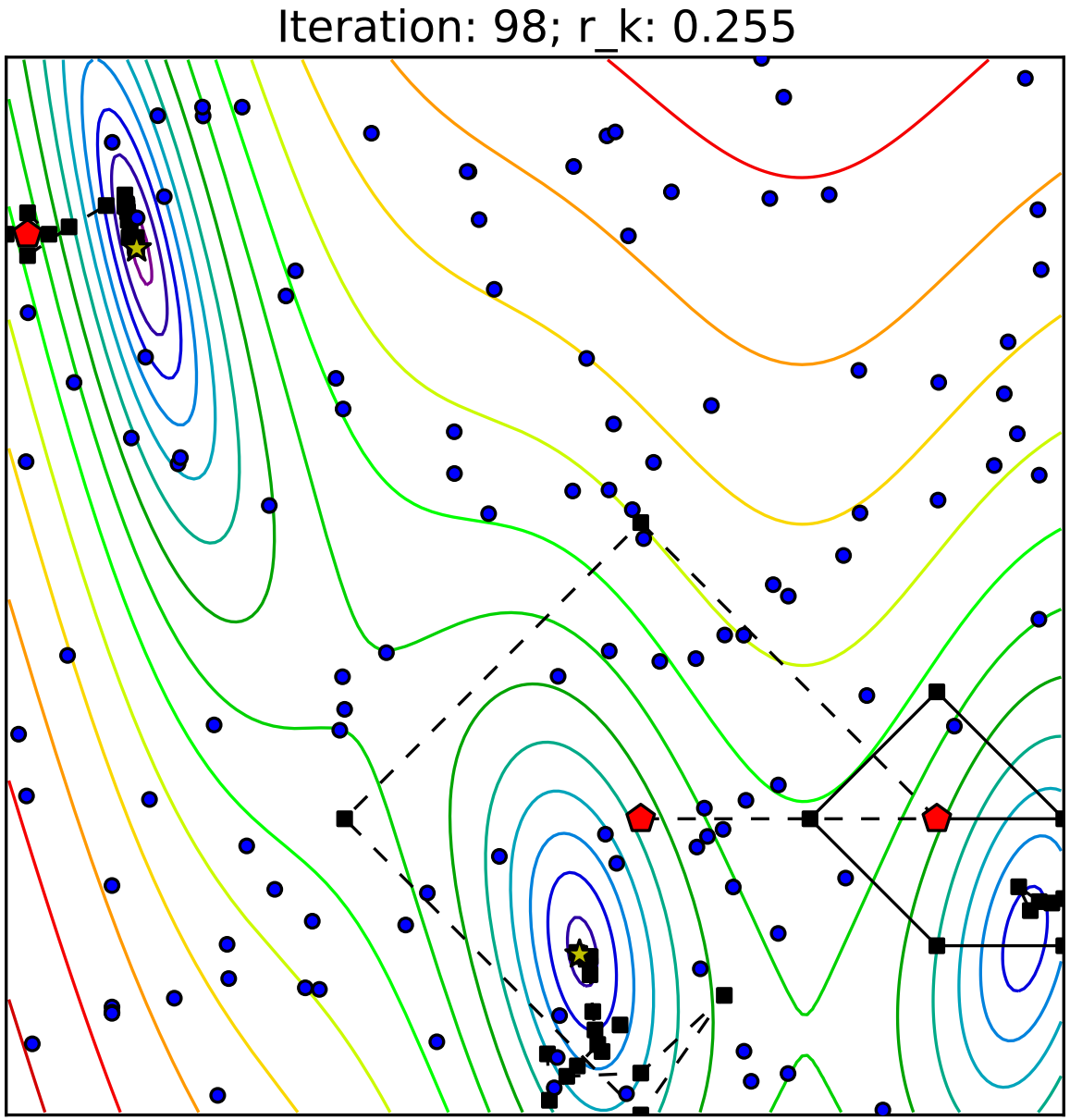

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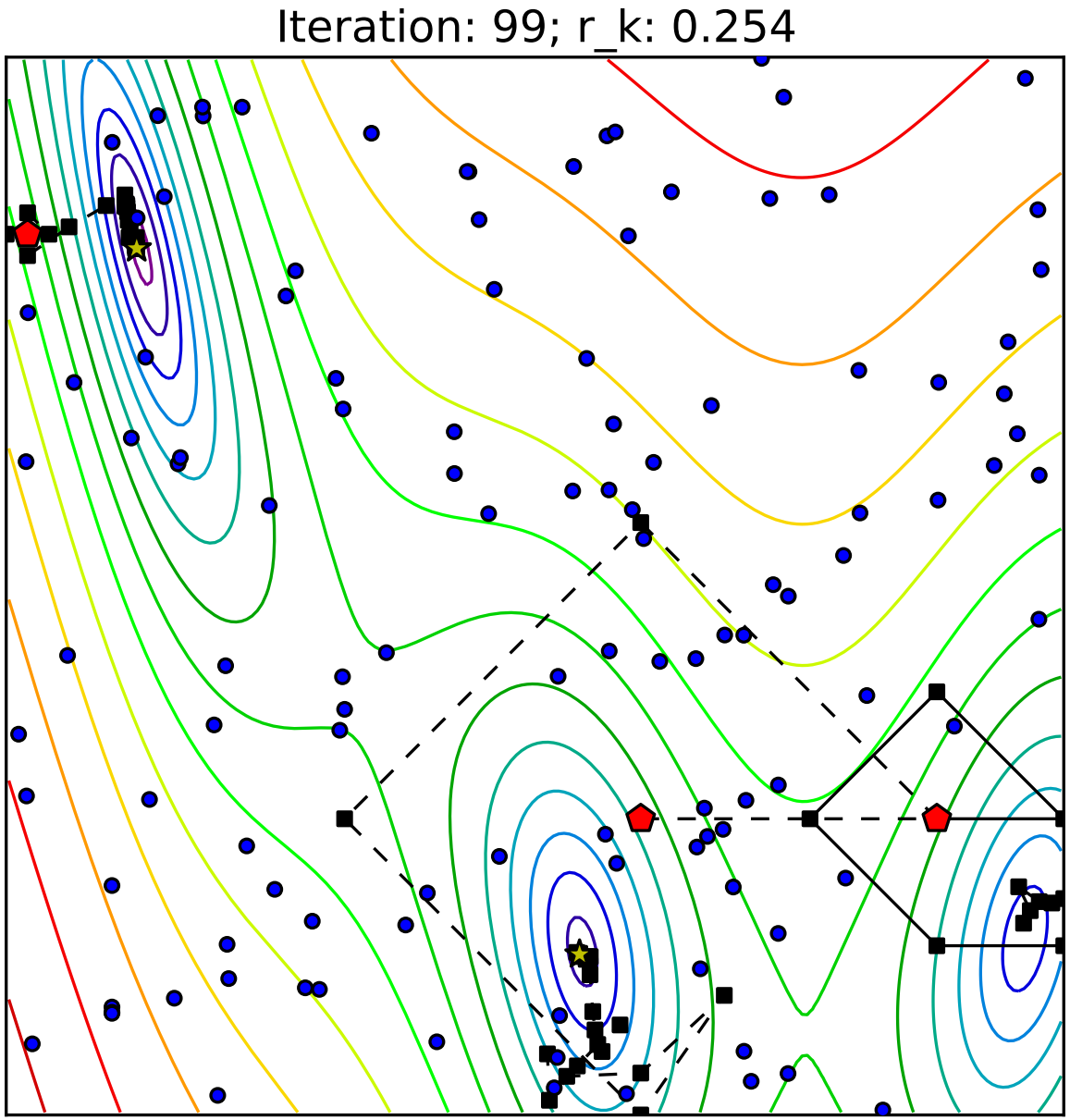

Properties of the local optimization method

Necessary:

- Honors a starting point
- Honors bound constraints

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Possibly beneficial:

- Can return multiple points of interest
- Reports solution quality/confidence at every iteration
- Can avoid certain regions in the domain
- Uses a history of past evaluations of f
- Uses additional points mid-run

Measuring Performance

Notation:

Let X^* be the set of all local minima of f.
Let $f^*_{(i)}$ be the ith smallest value $\{f(x^*)|x^* \in X^*\}$.
Let $x^*_{(i)}$ be the element of X^* corresponding to the value $f^*_{(i)}$.

The global minimum has been found at a level $\tau > 0$ at batch k if an algorithm it has found a point $\hat{x}$ satisfying:

$$f(\hat{x}) - f^*_{(1)} \leq (1 - \tau)\left(f(x_0) - f^*_{(1)}\right),$$

where x_0 is the starting point for problem p.

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The j best local minima have been found at a level $\tau > 0$ at batch k if:

$$\left|\left\{x^*_{(1)}, \ldots, x^*_{(\underline{j}-1)}\right\} \bigcap \left\{x^*_{(i)} : \exists x \in \mathcal{H}_k \text{ with } \left\|x - x^*_{(i)}\right\| \leq r_n(\tau)\right\}\right| = \underline{j} - 1$$

&

$$\left|\left\{x^*_{(\underline{j})}, \ldots, x^*_{(\bar{j})}\right\} \bigcap \left\{x^*_{(i)} : \exists x \in \mathcal{H}_k \text{ with } \left\|x - x^*_{(i)}\right\| \leq r_n(\tau)\right\}\right| \geq j - \underline{j} + 1,$$

where $\underline{j}$ and $\bar{j}$ are the smallest and largest integers such that $f^*_{(\bar{j})} = f^*_{(j)} = f^*_{(\underline{j})}$ and where $r_n(\tau) = \sqrt[n]{\frac{\tau \, \text{vol}(\mathcal{D})\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$.

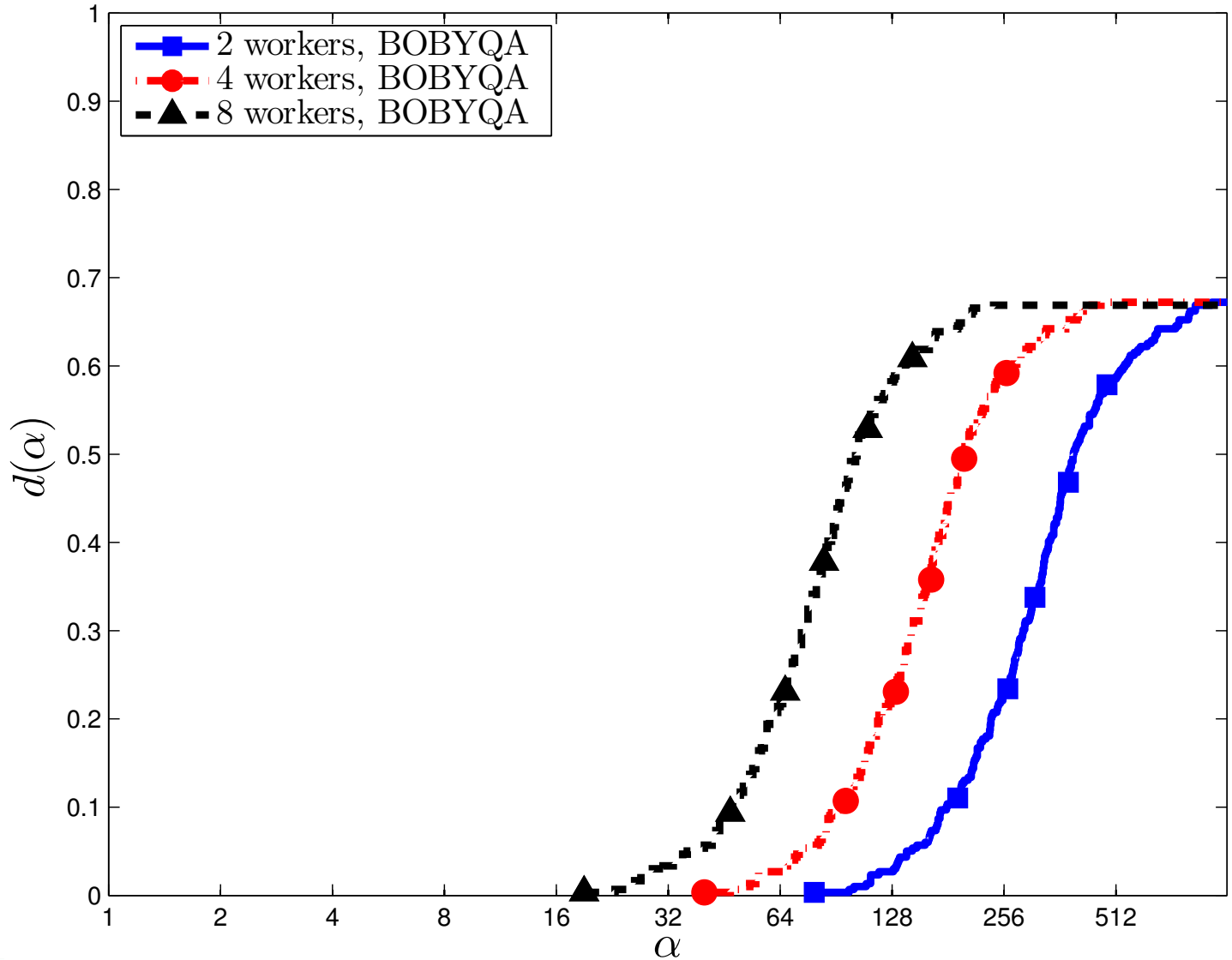
Problems considered

GKLS problem generator [Gaviano et al., "Algorithm 829" (TOMS, 2003)]

- 600 synthetic problems with known local minima
- $n = 2, \ldots, 7$
- 10 local minima in the unit cube with a unique global minimum
- 100 problems for each dimension
- 5 replications (different seeds) for each problem
- 5000 evaluations

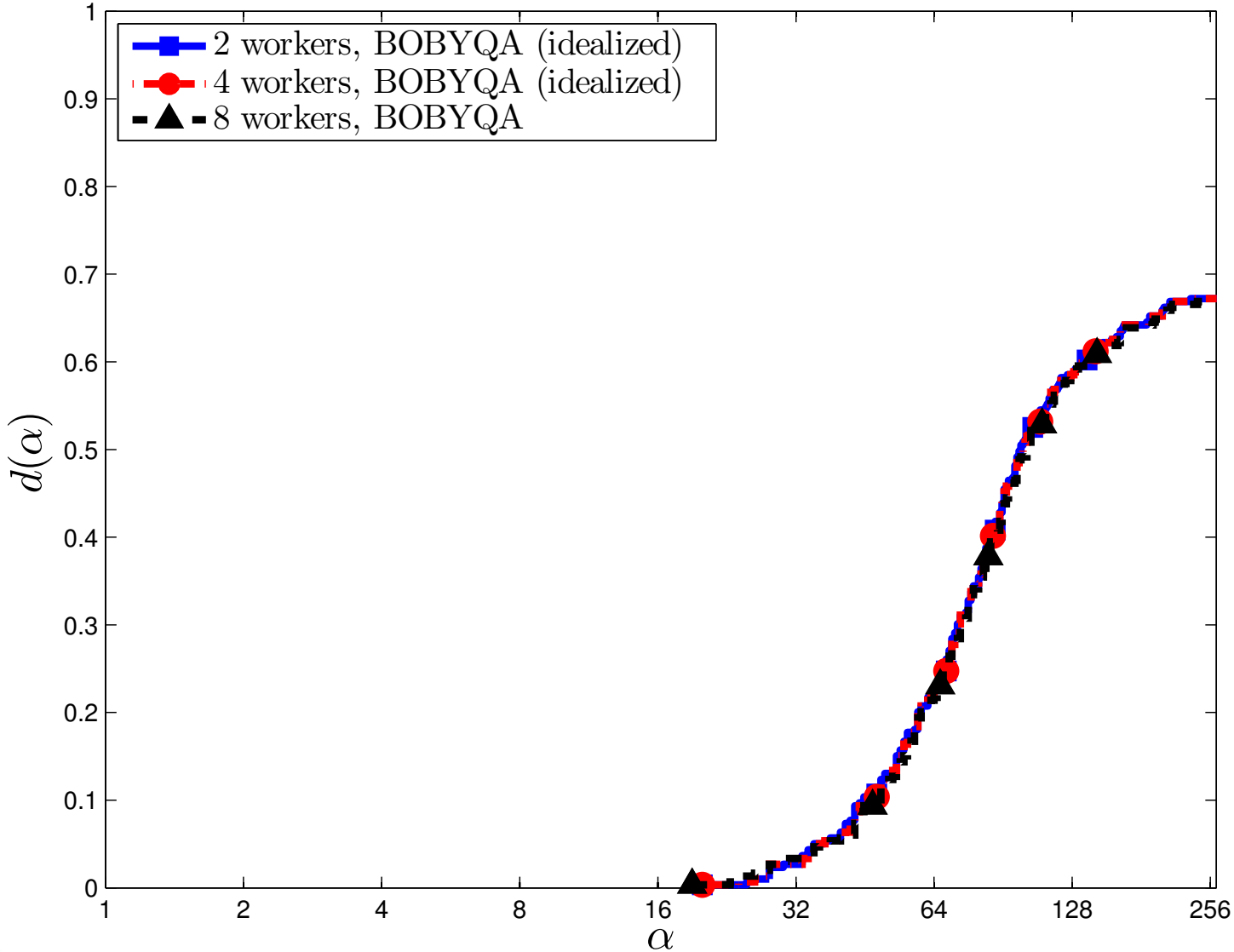
Data Profiles

Within $\sqrt[n]{\frac{10^{-3}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 7 best minima



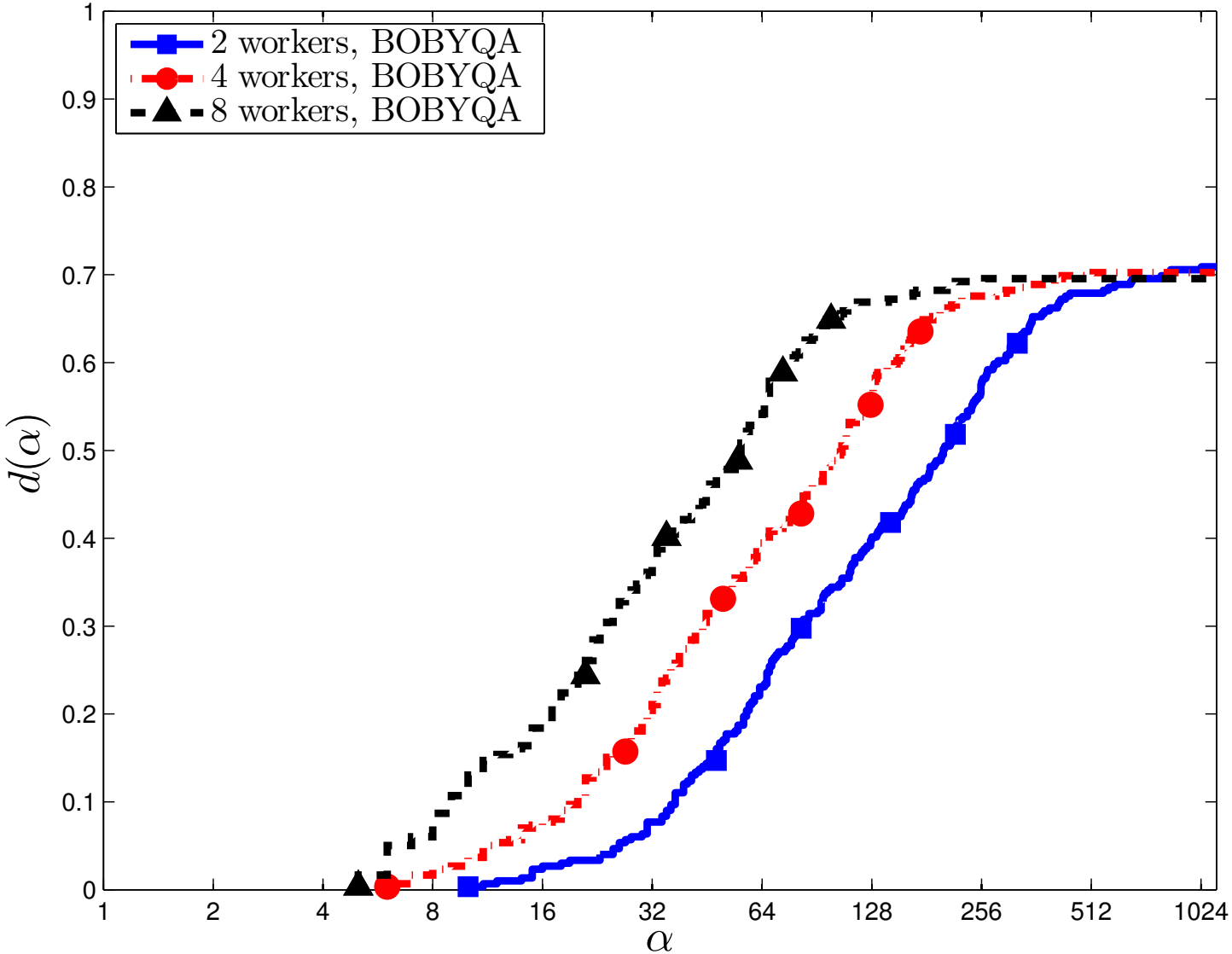
Data Profiles

Within $\sqrt[n]{\frac{10^{-3}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 7 best minima



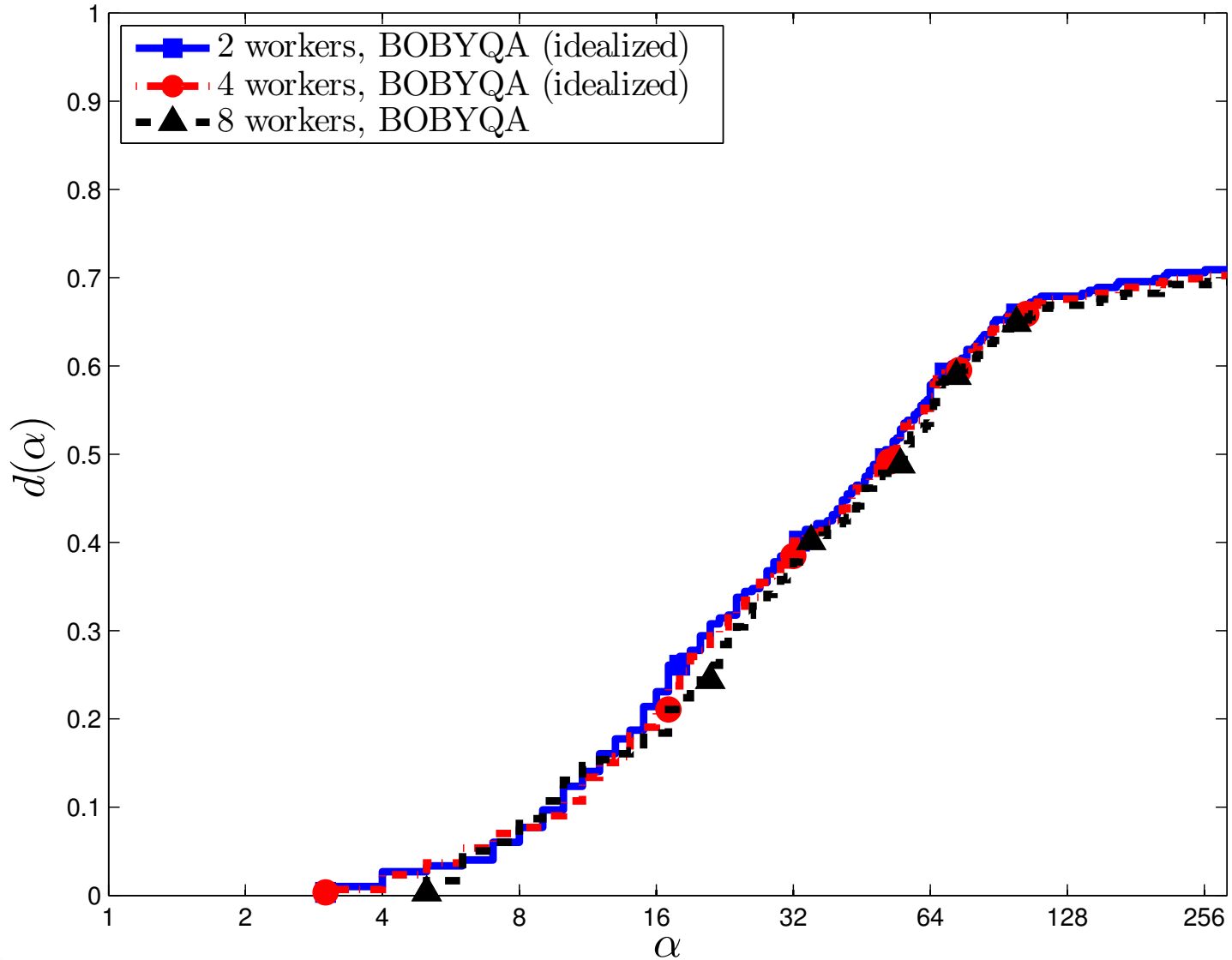
Data Profiles

Within $\sqrt[n]{\frac{10^{-4}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 3 best minima



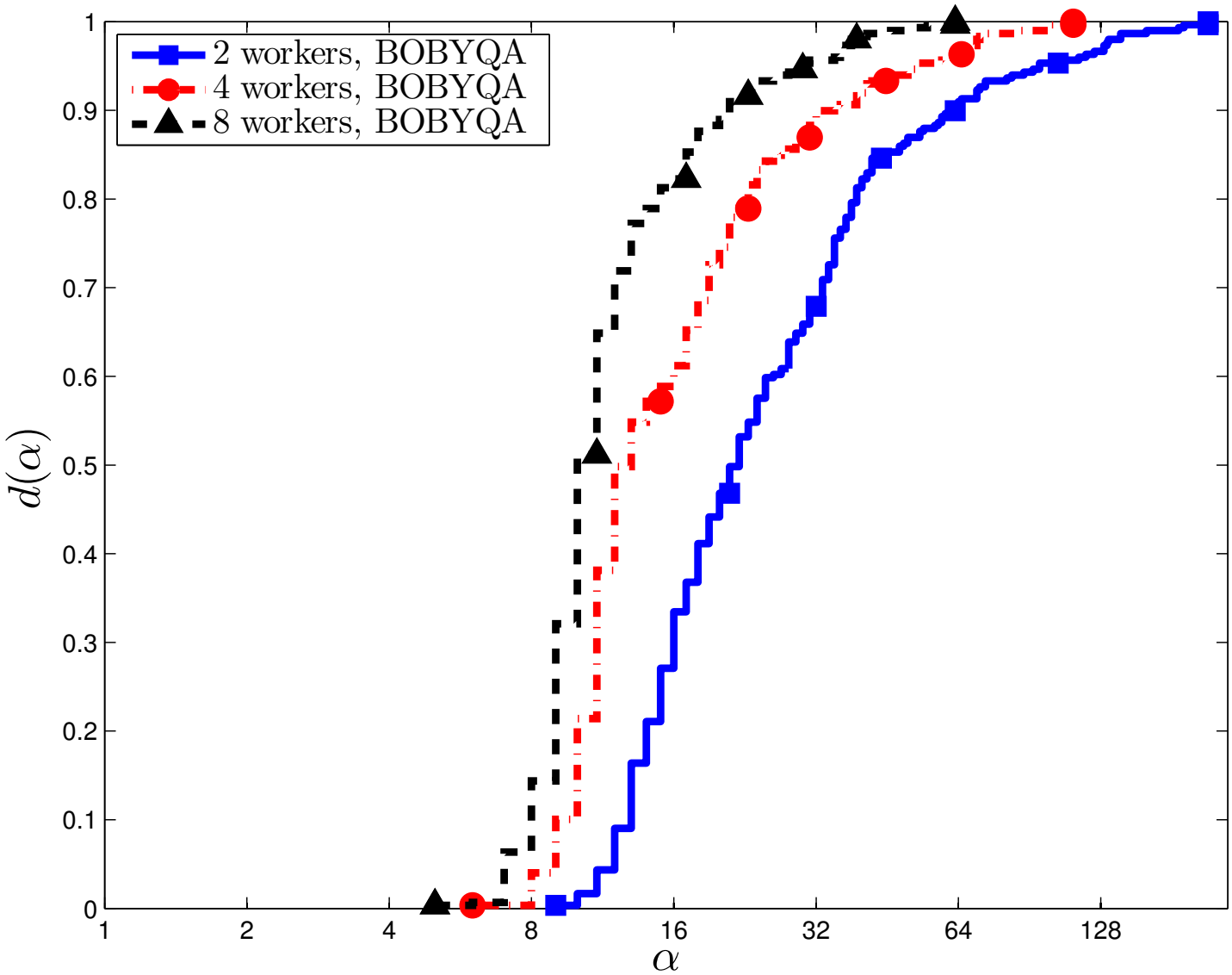
Data Profiles

Within $\sqrt[n]{\frac{10^{-4}\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$ of 3 best minima



Data Profiles

$$f(x) - f^*_{(1)} \leq (1 - 10^{-5}) \left(f(x_0) - f^*_{(1)} \right)$$



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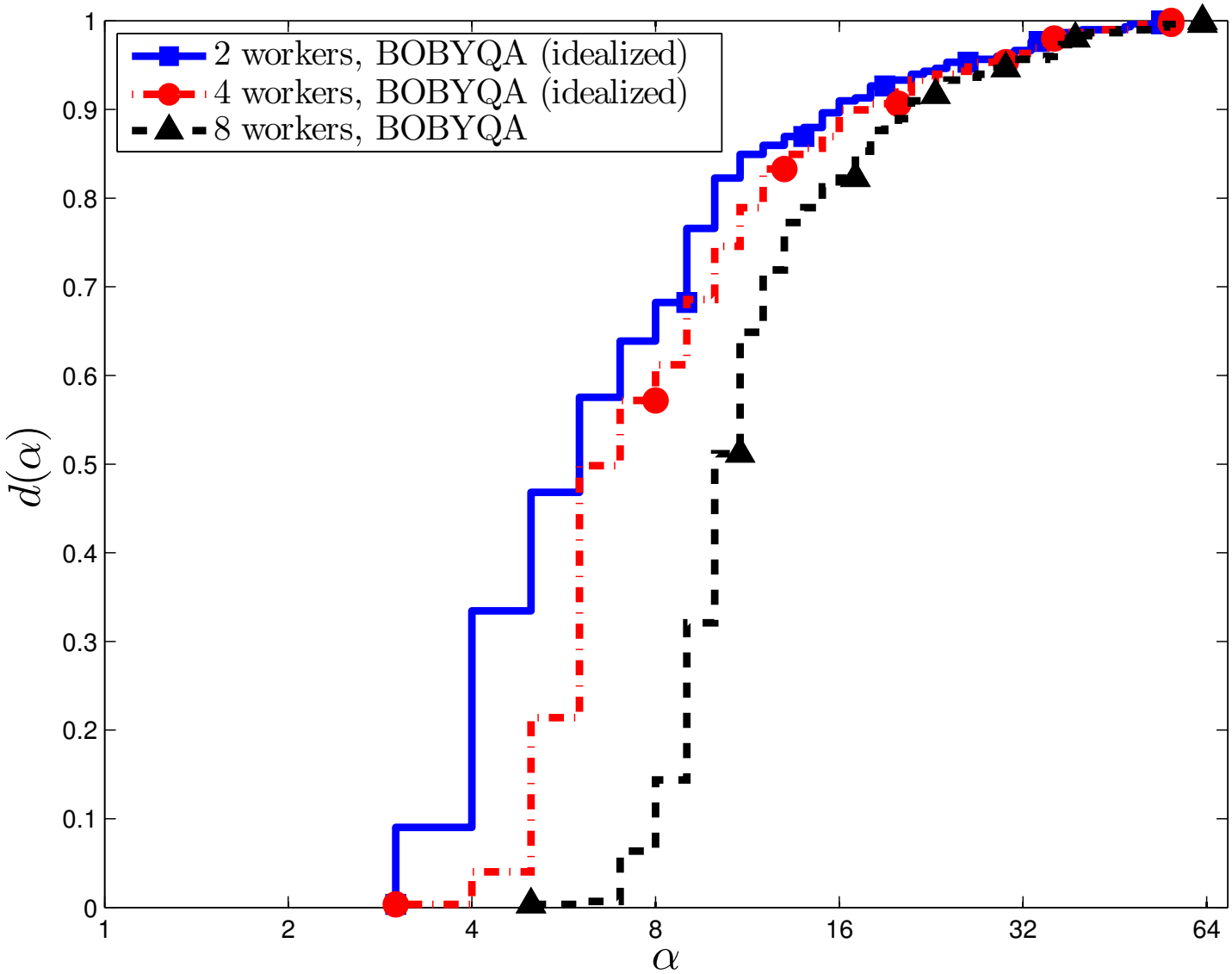

Closing Remarks

- `libEnsemble` is a software library to coordinate the concurrent evaluation of calculations.
- We have a growing set of use cases and examples.
- Let us know if you have examples you'd like to see.